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Title of Invention: _____

Inventors (please provide full names): _____

_____

Earliest Priority Filing Date: _____

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Online Time: _____	Other	_____	Other (specify)	_____

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L43  ANSWER 1 OF 16  HCAPLUS  COPYRIGHT 2003 ACS
AN   2003:319494  HCAPLUS
DN   138:316771
TI   Construction of modulators of protein kinase-associated
     signal transduction by using a hardware-software system comprising
     information on the three-dimensional structure of the kinase and
     application to drug screening and drug design
IN   Laster, Morris; Tobi, Dror
PA   Keryx Biopharmaceuticals, Inc., USA
SO   U.S. Pat. Appl. Publ., 79 pp.
     CODEN: USXXCO
DT   Patent
LA   English
IC   ICM C07K001-02
NCL  530023100
CC   7-3 (Enzymes)
     Section cross-reference(s): 1
FAN.CNT 1
     PATENT NO.         KIND  DATE          APPLICATION NO.   DATE
     ---------------    ----  --------      ---------------   --------
PI   US 2003078400      A1    20030424      US 2002-205302    20020726
PRAI US 2001-307939P    P     20010726
AB   The invention concerns a hardware-software system comprising information
     on the three-dimensional structure and nature of certain regions in
     protein kinases. The invention also concerns methods for
     screening for or synthesizing candidate chem. compds. for regulating
     kinase activity based on this information.
ST   protein kinase signal transduction modulator hardware
     software; drug screening design protein kinase signal
     transduction modulator
IT   Protein motifs
        (A-region; construction of modulators of protein
        kinase-assocd. signal transduction by using hardware-software
        system comprising information on 3-D structure of kinase and
        application to drug screening and drug design)
IT   Protein motifs
        (B4-B5 region; construction of modulators of protein
```

kinase-assocd. **signal** transduction by using hardware-software system comprising information on 3-D structure of kinase and application to drug screening and drug design)

IT **Protein** motifs
(HJ-loop; construction of modulators of **protein** kinase-assocd. **signal** transduction by using hardware-software system comprising information on 3-D structure of kinase and application to drug screening and drug design)

IT Human
(anticancer drugs for; construction of modulators of **protein** kinase-assocd. **signal** transduction by using hardware-software system comprising information on 3-D structure of kinase and application to drug screening and drug design)

IT Intestine, neoplasm
(colon, drug; construction of modulators of **protein** kinase-assocd. **signal** transduction by using hardware-software system comprising information on 3-D structure of kinase and application to drug screening and drug design)

IT Antitumor agents
Computer application
Computer program
Cytotoxic agents
Molecular modeling
Molecular recognition
Signal transduction, biological
(construction of modulators of **protein** kinase-assocd. **signal** transduction by using hardware-software system comprising information on 3-D structure of kinase and application to drug screening and drug design)

IT **Information systems**
(**data**, for 3-D coordinates; construction of modulators of **protein** kinase-assocd. **signal** transduction by using hardware-software system comprising information on 3-D structure of kinase and application to drug screening and drug design)

IT Cell morphology
(elongation, in drug screening assay; construction of modulators of **protein** kinase-assocd. **signal** transduction by using hardware-software system comprising information on 3-D structure of kinase and application to drug screening and design)

IT **Optical ROM disks**
(for 3-D coordinates; construction of modulators of **protein** kinase-assocd. **signal** transduction by using hardware-software system comprising information on 3-D structure of kinase and application to drug screening and drug design)

IT **Computer application**
(graphics; construction of modulators of **protein** kinase-assocd. **signal** transduction by using hardware-software system comprising information on 3-D structure of kinase and application to drug screening and drug design)

IT Apoptosis
Cell differentiation
Cell migration
Cell proliferation
Metabolism
Phosphorylation, biological
Secretion (process)
(in drug screening assay; construction of modulators of **protein** kinase-assocd. **signal** transduction by using hardware-software system comprising information on 3-D structure of kinase and application to drug screening and drug design)

IT Prostate gland
(neoplasm, drug; construction of modulators of **protein** kinase-assocd. **signal** transduction by using hardware-software

system comprising information on 3-D structure of kinase and application to drug screening and drug design)

IT Databases
(of 3-D coordinates; construction of modulators of **protein** kinase-assocd. **signal** transduction by using hardware-software system comprising information on 3-D structure of kinase and application to drug screening and drug design)

IT Hydration, chemical
(of exposed motifs; construction of modulators of **protein** kinase-assocd. **signal** transduction by using hardware-software system comprising information on 3-D structure of kinase and application to drug screening and drug design)

IT Phosphorylation, biological
(**protein**, in drug screening assay; construction of modulators of **protein** kinase-assocd. **signal** transduction by using hardware-software system comprising information on 3-D structure of kinase and application to drug screening and drug design)

IT Conformation
(**protein**; construction of modulators of **protein** kinase-assocd. **signal** transduction by using hardware-software system comprising information on 3-D structure of kinase and application to drug screening and drug design)

IT **Information systems**
(**storage**, for 3-D coordinates; construction of modulators of **protein** kinase-assocd. **signal** transduction by using hardware-software system comprising information on 3-D structure of kinase and application to drug screening and drug design)

IT Drug design
Drug screening
(structure-based; construction of modulators of **protein** kinase-assocd. **signal** transduction by using hardware-software system comprising information on 3-D structure of kinase and application to drug screening and drug design)

IT **Protein** motifs
(.alpha.D-region; construction of modulators of **protein** kinase-assocd. **signal** transduction by using hardware-software system comprising information on 3-D structure of kinase and application to drug screening and drug design)

IT 142008-39-5, **Protein** kinase A
RL: BSU (Biological study, unclassified); BUU (Biological use, unclassified); PRP (Properties); BIOL (Biological study); USES (Uses)
(C.alpha.; construction of modulators of **protein** kinase-assocd. **signal** transduction by using hardware-software system comprising information on 3-D structure of kinase and application to drug screening and drug design)

IT 9031-44-1, Kinase 140208-17-9, Lyn tyrosine kinase 372092-30-3, **Protein** kinase
RL: BSU (Biological study, unclassified); BUU (Biological use, unclassified); PRP (Properties); BIOL (Biological study); USES (Uses)
(construction of modulators of **protein** kinase-assocd. **signal** transduction by using hardware-software system comprising information on 3-D structure of kinase and application to drug screening and drug design)

L43 ANSWER 1 OF 16 HCAPLUS COPYRIGHT 2003 ACS
AN **2002:833111** HCAPLUS
DN **137:352439**
TI Biosequence information storage in binary format as mathematical summary values
IN Omori, Satoshi
PA Japan
SO PCT Int. Appl., 98 pp.
CODEN: PIXXD2

DT Patent
LA Japanese
IC ICM G06F017-30
ICS C12N015-00
CC 2-5 (History, Education, and Documentation)
Section cross-reference(s): 3
FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2002046761	A1	20020613	WO 2001-JP9801	20011109

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

	JP 2003041528	A2	20030213	JP 2001-120336	20010418
PRAI	JP 2001-120336	A	20010418		
	JP 2001-368002	A	20011130		
	JP 2000-117343	A	20000419		
	JP 2000-149122	A	20000519		

AB A method and device for storing biosequence information, nucleotide or amino acid sequence, in min. data storage space, by converting text format into binary format, is disclosed. Data are represented by math. summary values. Text data showing the sequences of a column of nucleotides constituting the DNA of a std. sample E are converted into binary data in accordance with a definite conversion rule. Then the binary data are divided into partial data (A(i,j)) of m bits (m.gtoreq.16) having a plural no. of rows and a plural no. of columns. Next, the partial data (A(i,j)) of each row are computed in the row-sequence direction on Galois field GF (2m) to det. the first parity group (B1(i) to B3(i)). Then, the partial data (A(i,j)) of each column are computed in the sequence direction on Galois field GF (2m) to det. the second parity group (C1(j) to C3(j)). From these parity data, the sequences of the nucleotides are approx. represented. Computer readable memory storage devices, such as DVD-ROM, or CD-ROM, are claimed.

ST app recording storage sequence computer text binary data conversion; sequence information storage binary format math summary value

IT Computers
DNA sequences
Information, biological
Magnetic memory devices
Optical ROM disks
Protein sequences
RNA sequences
(biosequence information storage in binary format as math. summary values)

IT **Information systems**
(**retrieval, computerized;** biosequence information **storage** in binary format as math. summary values)

IT **Information systems**
(**storage, computerized;** biosequence information **storage** in binary format as math. summary values)

IT **Mathematical methods**
(text to binary data conversion; biosequence information storage in binary format as math. summary values)

IT 474443-04-9, 1: PN: WO0203676l SEQID: 1 unclaimed DNA 474443-10-2, 2: PN: WO0203676l SEQID: 2 unclaimed DNA
PL: PPP (Properties)
(unclaimed nucleotide sequence; biosequence information storage in

binary format as math. summary values)
IT 474443-11-3
RL: PRP (Properties)
(unclaimed **protein** sequence; biosequence information storage in binary format as math. summary values)
RE.CNT 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD
RE
(1) Casio Computer Co Ltd; JP 06-162096 A 1994
(2) Fukuda, M; Dai 22 Kai Johs Kagaku Toronkai Dai 27 Kai Kozo Kassei Sokan Symposium Koen Yoshishu 1999, P84
(3) International Business Machines Corp; JP 06-348760 A 1994
(4) International Business Machines Corp; JP 08-055176 A 1996
(5) International Business Machines Corp; US 5810268 A 1996
(6) Mitsubishi Electric Corp; JP 03-63876 A 1991
(7) Nec Corp; JP 06-320834 A 1996
(8) Nippon Telegraph & Telephone Corp; JP 05-143472 A 1993
(9) Robson, B; Computer Applications in Biosciences 1992, P283 HCAPLUS
(10) Tokyo Electric Co Ltd; JP 04-54656 A 1992

L43 ANSWER 3 OF 16 HCAPLUS COPYRIGHT 2003 ACS
AN **2002:778603** HCAPLUS
DN **137:259621**
TI Method and apparatus for improving the performance of microanalytic and microsynthetic procedures
IN Howard, John K.
PA Matsushita Electric Industrial Co., Ltd., Japan
SO U.S. Pat. Appl. Publ., 9 pp.
CODEN: USXXCO
DT Patent
LA English
IC ICM C12Q001-68
ICS G01N033-53; G01N033-543; G11B007-24; G06F019-00; C12M001-34
NCL 435006000
CC **9-1 (Biochemical Methods)**
Section cross-reference(s): 14
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI US 2002146699	A1	20021010	US 2001-827895	20010409
PRAI US 2001-827895		20010409		

AB In a first exemplary embodiment, the present invention relates to an app. for performing an assay comprising a micro-system platform, a CD-ROM device and an information processor, where the CD-ROM device under control of the information processor is capable of reading and writing data to the micro-system platform. The micro-system platform comprises a first section for storing data in a continuous circular data band, which is disposed in an inner portion of the micro-system platform, and a second section including at least one assay, which is formed in an outer portion of the micro-system platform. During operation, the CD-ROM device retrieves and stores data related to the performance of the assay in the circular data band. The information processor is operative for controlling the CD-ROM device in accordance with the data retrieved from the circular data band, and for analyzing the results of the assay.
ST app performance microanalysis microsynthetic
IT Disks
(Bioanal.; method and app. for improving performance of microanalytic and microsynthetic procedures)
IT Interface
(Flat planar; method and app. for improving performance of microanalytic and microsynthetic procedures)
IT Analysis
(clin.; method and app. for improving performance of microanalytic and microsynthetic procedures)

IT **Information systems**
(**data**; method and app. for improving performance of microanalytic and microsynthetic procedures)
IT Aging, animal
Analytical apparatus
Diagnosis
Human
Information systems
Optical ROM disks
Statistical analysis
(method and app. for improving performance of microanalytic and microsynthetic procedures)
IT **Information systems**
(**retrieval**; method and app. for improving performance of microanalytic and microsynthetic procedures)
IT **Information systems**
(**storage**; method and app. for improving performance of microanalytic and microsynthetic procedures)

L43 ANSWER 4 OF 16 HCAPLUS COPYRIGHT 2003 ACS
AN **2002:637867** HCAPLUS
DN **137:165843**
TI Network for evaluating data obtained in a biochip measurement device
IN Abraham-fuchs, Klaus; Hengerer, Arne; Gallahue, Kieran T.; Gosch, Greg; O'Connell, James P.; Windhab, Norbert
PA Siemens Aktiengesellschaft, Germany; Nanogen, Inc.
SO PCT Int. Appl., 18 pp.
CODEN: PIXXD2
DT Patent
LA English
IC ICM C12Q001-68
CC **9-16** (**Biochemical Methods**)
Section cross-reference(s): 14
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 2002064826	A2	20020822	WO 2002-EP1565	20020214
W: CA, JP				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR				
PRAI US 2001-784720	A	20010215		

AB In a method and a network for evaluating medical data in a clin. study, biochips contg. patient samples with multiple biomol. markers are tested in a no. of point of care test devices resp. at point of care sites. Each test of each biochip sample produces a diagnostic result, which is entered into the electronic patient record for the patient who produced the sample. A follow-up examn. is subsequently conducted for each patient, and the results of the follow-up examn. are also entered into that patient's electronic patient record. The follow-up results indicate whether the diagnostic test result was a false pos., a false neg. or correct. The follow-up data and the original diagnostic results from all point of care sites are electronically transmitted to a remote server, which has access to an expert system which uses the test results and the follow-up data to automatically devise a measurement protocol for a selected pathol.
ST network biochip device
IT **Information systems**
(Electronic; **network** for evaluating **data** obtained in a biochip measurement device)
IT Computers
(Servers; network for evaluating data obtained in a biochip measurement device)
IT Clinical analyzers

(biochips; network for evaluating data obtained in a biochip measurement device)
IT Analysis
(clin.; network for evaluating data obtained in a biochip measurement device)
IT **Information systems**
(**data**, Medical; **network** for evaluating **data** obtained in a biochip measurement device)
IT **Information systems**
(**data**; **network** for evaluating **data** obtained in a biochip measurement device)
IT **Computer application**
(expert systems; network for evaluating data obtained in a biochip measurement device)
IT Biochemical molecules
Biomarkers (biological responses)
Communication
Diagnosis
Disease, animal
Human
Memory devices
Samples
(network for evaluating data obtained in a biochip measurement device)
IT **Information systems**
(**network**; **network** for evaluating **data** obtained in a biochip measurement device)

L43 ANSWER 5 OF 16 HCAPLUS COPYRIGHT 2003 ACS
AN **2002:595322** HCAPLUS
DN **137:121955**
TI Systems and computer software products for comparing microarray spot intensities
IN Partell, Daniel M.; Liu, Wei-min
PA USA
SO U.S. Pat. Appl. Publ., 16 pp.
CODEN: USXXCO
DT Patent
LA English
IC ICM G06K009-00
ICS G06F019-00; G01N033-48; G01N033-50; G06K009-34
NCL 382129000
CC **9-16** (**Biochemical Methods**)
Section cross-reference(s): 3
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI US 2002106117	A1	20020808	US 2000-737536	20001213
PRAI US 2000-737536		20001213		

AB Methods, systems and computer software products are provided for analyzing gene expression data using pixel intensities.
ST system computer software product comparing microarray spot intensity
IT **Information systems**
(**data**; systems and computer software products for comparing microarray spot intensities)
IT Gene
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(expression; systems and computer software products for comparing microarray spot intensities)
IT **Information systems**
(**storage**; systems and computer software products for comparing microarray spot intensities)
IT **Computer program**
DNA microarray technology

Mathematical methods
Memory devices
Microarray technology
Statistical analysis
(systems and computer software products for comparing microarray spot intensities)
IT Nucleic acids
Oligonucleotides
cDNA
RL: ANT (Analyte); ANST (Analytical study)
(systems and computer software products for comparing microarray spot intensities)
IT Probes (nucleic acid)
RL: ARG (Analytical reagent use); ANST (Analytical study); USES (Uses)
(systems and computer software products for comparing microarray spot intensities)

L43 ANSWER 6 OF 16 HCAPLUS COPYRIGHT 2003 ACS
AN **2002:522146** HCAPLUS
DN **137:59914**
TI Database system and method useful for predicting the effect of amino acid substitutions on **protein** structure and stability
IN Edelman, Marvin; Eyal, Eran; Najmanovich, Rafael; Sobolev, Vladimir
PA Yeda Research and Development Co. Ltd., Israel
SO PCT Int. Appl., 34 pp.
CODEN: PIXXD2
DT Patent
LA English
IC ICM G01N033-48
CC **9-16** (**Biochemical Methods**)
Section cross-reference(s): 6
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 2002054063	A1	20020711	WO 2001-IL1193	20011204

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PRAI US 2001-259511P P 20010104
AB A method of predicting an effect of a specific amino acid substitution, or mutation, on a structure or stability of a **protein** of interest is disclosed, as well as hardware for implementing the method. The method is executed, at least in part, by a computer and is effected by (a) selecting at least one pair of structurally characterized **proteins** or portions of **proteins**, members of the at least one pair differing in at least the specific amino acid substitution; and (b) extg. data from the members, the data being useful in predicting the effect of the specific amino acid substitution on at least one structural parameter of at least a portion of the **protein** of interest.
ST database system predicting amino acid substitution **protein** structure stability
IT **Computer application**
Computer program
Computers
Databases
Information systems

Internet
Memory devices
Molecular orientation
Molecular structure
Optical ROM disks
(database system and method useful for predicting effect of amino acid substitutions on **protein** structure and stability)
IT Amino acids, properties
Proteins
RL: PRP (Properties)
(database system and method useful for predicting effect of amino acid substitutions on **protein** structure and stability)
IT Conformation
(**protein**; database system and method useful for predicting effect of amino acid substitutions on **protein** structure and stability)
IT **Information systems**
(**searching**; database system and method useful for predicting effect of amino acid substitutions on **protein** structure and stability)
RE.CNT * THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD
RE
(1) Domingues; Proteins:Structure, Function, and Genetic Suppl 1999, V3, P112
(2) Dubchak; Proceedings of the National Academy of Sciences 1995, V92, P8700 HCAPLUS
(3) Fischer; Protein Science 1996, V5, P947 HCAPLUS
(4) Freire; US 6226603 B1 2001
(5) Hopp; Proceedings of the National Academy of Sciences 1981, V78(6), P3824 HCAPLUS
(6) Parker; Journal of Computer-Aided Molecular Design 1994, V8, P195 HCAPLUS

L43 ANSWER 7 OF 16 HCAPLUS COPYRIGHT 2003 ACS
AN **2002:516579** HCAPLUS
DN **137:59853**
TI Remotely programmable matrices with memories
IN Nova, Michael P.; Senyei, Andrew E.
PA Discovery Partners International, Inc., USA
SO U.S., 35 pp., Cont.-in-part of U.S. Ser. No. 428,662.
CODEN: USXXAM
DT Patent
LA English
IC ICM G01N015-06
ICS G01N033-53; C12Q001-68; A61K038-00
NCL 435/2069100
CC **9-1** (**Biochemical Methods**)
Section cross-reference(s): 7, 80
FAN.CNT 20

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 6416714	B1	20020709	US 1995-444466	19950607
	US 5741462	A	19980421	US 1995-429062	19950425
	US 5874214	A	19990223	US 1995-538367	19951003
	US 6025129	A	20000215	US 1995-567746	19951205
	CA 2216645	AA	19961121	CA 1996-2216645	19960425
	WO 9636436	A1	19961121	WO 1996-US6145	19960425
	W: AL, AM, AT, AU, AZ, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI				
	RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN				
	EP 822861	A1	19980211	EP 1996-916437	19960425
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,				

IE, SI, LT, LV, FI

	CN 1181720	A	19980513	CN 1996-193774	19960425
	JP 11511338	T2	19990924	JP 1996-530462	19960425
	AU 9659185	A1	19961129	AU 1996-59185	19960501
	AU 707444	B2	19990708		
	US 6100026	A	20000808	US 1996-633410	19960610
	US 6331658	B1	20011220	US 1996-669352	19960624
	US 6284459	B1	20010904	US 1996-711426	19960905
	US 6017496	A	20000125	US 1996-709435	19960906
	US 5961925	A	19991005	US 1996-723423	19960930
	US 6329139	B1	20011211	US 1997-912094	19970811
	US 6340566	B1	20020122	US 1998-71022	19980422
PRAI	US 1995-418662	A2	19950407		
	US 1995-434504	A2	19950607		
	US 1995-473660	A	19950607		
	US 1995-480147	A2	19950607		
	US 1995-480196	A	19950607		
	US 1995-484486	A	19950607		
	US 1995-484504	A2	19950607		
	US 1995-538387	A2	19951003		
	US 1996-567746	A	19961205		
	US 1996-639813	A	19960425		
	WO 1996-US6145	W	19960425		
	US 1996-633410	A2	19960610		
	US 1996-669352	A2	19960624		
	US 1996-711426	A2	19960905		
	US 1996-709435	A2	19960906		
	US 1996-723423	A2	19960930		
	WO 1996-US15939	A3	19961003		
	US 1996-736703	B2	19961007		
	US 1996-743984	A2	19961028		
	US 1996-741685	B1	19961031		
	US 1997-957806	B2	19971022		
	US 1997-976153	B2	19971727		
	US 1997-945053	B2	19971021		

AB Combinations, called matrixes with memories, of matrix materials with remotely addressable or remotely programmable recording devices that contain at least one data storage unit are provided. The matrix materials are those that are used in as supports in solid phase chem. and biochem. syntheses, immunoassays and hybridization reactions. The data storage units are preferably non-volatile antifuse memories. By virtue of this combination, mols. and biol. particles, such as phage and viral particles and cells, that are in proximity or in phys. contact with the matrix combination can be labeled by programming the memory with identifying information and can be identified by retrieving the stored information. Combinations of matrix materials, memories, and linked mols. and biol. materials are also provided. The combinations have a multiplicity of applications, including combinatorial chem., isolation and purifn. of target macromols., capture and detection of macromols. for anal. purposes, selective removal of contaminants, enzymic catalysis, chem. modification and other uses.

ST remotely programmable matrixes memory; memory device program app array combinatorial phage library

IT Electromagnetic field
(as tags; remotely programmable matrixes with memories)

IT Chromatographs
(columns; remotely programmable matrixes with memories)

IT Containers
(contg. the matrixes with memories; remotely programmable matrixes with memories)

IT **Information systems**
(**data;** remotely programmable matrixes with memories)

IT Immunoassay

(immunoblotting; remotely programmable matrixes with memories)
IT Analytical apparatus
Antifuses
Combinatorial chemistry
Combinatorial library
Computer application
DNA microarray technology
Immobilization, molecular
Immunoassay
Memory devices
Microtiter plates
Northern blot hybridization
Nucleic acid hybridization
Optical detectors
Particles
Phage display library
Process automation
Solid phase synthesis
Southern blot hybridization
Test tubes
Vials
(remotely programmable matrixes with memories)
IT DNA
Proteins
RNA
RL: ANT (Analyte); CRT (Combinatorial reactant); RCT (Reactant); ANST (Analytical study); CMBT (Combinatorial study); RACT (Reactant or reagent)
(remotely programmable matrixes with memories)
IT 9004-70-0, Nitrocellulose
RL: DEV (Device component use); USES (Uses)
(remotely programmable matrixes with memories)
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L43 ANSWER 9 OF 16 HCAPLUS COPYRIGHT 2003 ACS
AN **2002:332714** HCAPLUS
DN **136:337373**
TI Computer systems and methods for hierarchical cluster analysis of large sets of biological data including highly dense gene array data
IN Fahy, Eoin D.
PA USA
SO U.S. Pat. Appl. Publ., 31 pp.
CODEN: USXXCO
DT Patent
LA English
IC ICM G01N033-48
ICS G01N019-06; G06F007-00
NCL 702019000
CC **9-16** (**Biochemical Methods**)
Section cross-reference(s): 3
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 2002052692	A1	20020502	US 1999-397580	19990915
PRAI	US 1999-397580		19990915		

AB A system and corresponding method analyzes biol. data for sets of test subjects such as gene arrays of group test subjects into clusters and order the clusters into a hierarchy based on similarities and differences of biol. data corresponding to the test subjects. A combination of nonhierarchical clustering and hierarchical clustering methods is used to efficiently and effectively perform hierarchical clustering of such biol. data as highly dense gene arrays contg. many thousand test subjects such as genes. First the test subjects are nonhierarchically clustered according to similarities and differences of their biol. data as detd. by distance techniques. Representative values, such as mean values, of the biol. data are detd. for each nonhierarchical cluster of test subjects. These representative values are then used to hierarchically cluster the nonhierarchical clusters. Biol. data for each test subject is displayed in a row of a table. The rows of the table are arranged by the nonhierarchical clustering and further by the hierarchical clustering. Each value of the biol. data is color coded according to its value to display patterns in the hierarchically clustered biol. data.
ST computer system hierarchical cluster analysis biol dense gene array
IT **Mathematical methods**
(Block; computer systems and methods for hierarchical cluster anal. of large sets of biol. data including highly dense gene array data)
IT **Mathematical methods**
(Chebychev distance; computer systems and methods for hierarchical cluster anal. of large sets of biol. data including highly dense gene array data)
IT **Mathematical methods**
(Chebychev; computer systems and methods for hierarchical cluster anal. of large sets of biol. data including highly dense gene array data)

IT **Mathematical methods**
(City-block; computer systems and methods for hierarchical cluster anal. of large sets of biol. data including highly dense gene array data)

IT Education
(Computer-readable instructions; computer systems and methods for hierarchical cluster anal. of large sets of biol. data including highly dense gene array data)

IT **Mathematical methods**
(Cosine; computer systems and methods for hierarchical cluster anal. of large sets of biol. data including highly dense gene array data)

IT **Mathematical methods**
(Euclidean distance detns.; computer systems and methods for hierarchical cluster anal. of large sets of biol. data including highly dense gene array data)

IT **Mathematical methods**
(Euclidean; computer systems and methods for hierarchical cluster anal. of large sets of biol. data including highly dense gene array data)

IT Computers
(Hard drives; computer systems and methods for hierarchical cluster anal. of large sets of biol. data including highly dense gene array data)

IT **Mathematical methods**
(Isodata; computer systems and methods for hierarchical cluster anal. of large sets of biol. data including highly dense gene array data)

IT **Mathematical methods**
(Manhattan distance; computer systems and methods for hierarchical cluster anal. of large sets of biol. data including highly dense gene array data)

IT **Mathematical methods**
(Minkowski; computer systems and methods for hierarchical cluster anal. of large sets of biol. data including highly dense gene array data)

IT **Mathematical methods**
(Parallel threshold; computer systems and methods for hierarchical cluster anal. of large sets of biol. data including highly dense gene array data)

IT **Mathematical methods**
(Pearson correlation; computer systems and methods for hierarchical cluster anal. of large sets of biol. data including highly dense gene array data)

IT **Mathematical methods**
(Percent disagreement; computer systems and methods for hierarchical cluster anal. of large sets of biol. data including highly dense gene array data)

IT **Computer program**
(Perl script language; computer systems and methods for hierarchical cluster anal. of large sets of biol. data including highly dense gene array data)

IT **Mathematical methods**
(Power distance; computer systems and methods for hierarchical cluster anal. of large sets of biol. data including highly dense gene array data)

IT **Mathematical methods**
(Sequential threshold; computer systems and methods for hierarchical cluster anal. of large sets of biol. data including highly dense gene array data)

IT **Mathematical methods**
(Squared Euclidean; computer systems and methods for hierarchical cluster anal. of large sets of biol. data including highly dense gene array data)

IT Construction materials
(blocks; computer systems and methods for hierarchical cluster anal. of large sets of biol. data including highly dense gene array data)

IT Color
(coding; computer systems and methods for hierarchical cluster anal. of large sets of biol. data including highly dense gene array data)
IT Optical imaging devices
(color, monitors; computer systems and methods for hierarchical cluster anal. of large sets of biol. data including highly dense gene array data)
IT Agglomeration
Clusters
Computer application
Computer program
Computers
Configuration
DNA microarray technology
Databases
Human
Information, biological
Optical ROM disks
Optimization
Statistical analysis
(computer systems and methods for hierarchical cluster anal. of large sets of biol. data including highly dense gene array data)
IT Gene
Proteins
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(computer systems and methods for hierarchical cluster anal. of large sets of biol. data including highly dense gene array data)
IT **Information systems**
(**data**, Biol.; computer systems and methods for hierarchical cluster anal. of large sets of biol. **data** including highly dense gene array **data**)
IT Gene
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(expression; computer systems and methods for hierarchical cluster anal. of large sets of biol. data including highly dense gene array data)
IT **Cluster analysis**
(hierarchical; computer systems and methods for hierarchical cluster anal. of large sets of biol. data including highly dense gene array data)
IT **Mathematical methods**
(k-means; computer systems and methods for hierarchical cluster anal. of large sets of biol. data including highly dense gene array data)
IT **Computer program**
(spreadsheet; computer systems and methods for hierarchical cluster anal. of large sets of biol. data including highly dense gene array data)
IT **Information systems**
(**storage**; computer systems and methods for hierarchical cluster anal. of large sets of biol. **data** including highly dense gene array **data**)
IT Audiovisual aids
(tables; computer systems and methods for hierarchical cluster anal. of large sets of biol. data including highly dense gene array data)

L43 ANSWER 9 OF 16 HCAPLUS COPYRIGHT 2003 ACS
AN **2002:165034** HCAPLUS
DN **136:213153**
TI Remotely programmable matrices with memories
IN Nova, Michael P.; Senyei, Andrew E.
PA Discovery Partners International, Inc., USA
SO U.S., 29 pp., Cont.-in-part of U. S. 5,741,462.
CODEN: USXXAM

DT Patent
LA English
IC ICM C12M001-34
ICS C12Q004-68; G01N033-53; C07H021-04; C07F014-00
NCL 435287100
CC **9-1 (Biochemical Methods)**
Section cross-reference(s): 7, 80
FAN.CNT 20

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 6052854	B1	20000425	US 1995-440147	19950607
	US 5741462	A	19980421	US 1995-438063	19950425
	US 5874214	A	19990223	US 1995-538387	19951003
	US 6001229	A	19991214	US 1995-567746	19951205
	CA 2216645	AA	19961121	CA 1996-2216645	19960425
	WO 9636436	A1	19961121	WO 1996-US6145	19960425
	W: AL, AM, AT, AU, AZ, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI				
	RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN				
	EP 822861	A1	19980211	EP 1996-916437	19960425
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI				
	CN 1191728	A	19980819	CN 1996-193874	19960425
	JP 11511238	T2	19990924	JP 1996-535062	19960425
	AU 9656165	A1	19961129	AU 1996-56165	19960501
	AU 707444	B2	19990708		
	US 6100026	A	20000808	US 1996-638410	19960610
	US 6319668	B1	20011120	US 1996-664752	19960614
	US 6294459	B1	20010904	US 1996-711426	19960905
	US 6017496	A	20000125	US 1996-704435	19960906
	US 5961923	A	19991005	US 1996-723423	19960930
	US 6329139	B1	20011211	US 1997-912906	19970811
	US 6340588	B1	20020122	US 1998-51022	19980922
PRAI	US 1995-418662	A2	19950425		
	US 1995-164504	A2	19950607		
	US 1995-473660	A	19950607		
	US 1995-480147	A2	19950607		
	US 1995-480196	A	19950607		
	US 1995-484486	A	19950607		
	US 1995-484504	A2	19950607		
	US 1995-538387	A2	19951003		
	US 1995-567746	A	19951205		
	US 1996-639813	A	19960402		
	WO 1996-US6145	W	19960425		
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	US 1996-669252	A2	19960614		
	US 1996-711426	A2	19960905		
	US 1996-709435	A2	19960906		
	US 1996-723423	A2	19960930		
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	US 1997-857800	B2	19970122		
	US 1997-926253	B2	19970827		
	US 1997-945053	B2	19971021		

AB Combinations, called matrixes with memories, of matrix materials with remotely addressable or remotely programmable recording devices that contain at least one data storage unit are provided. The matrix materials are those that are used in as supports in solid phase chem. and biochem.

syntheses, immunoassays and hybridization reactions. The data storage units are preferably nonvolatile antifuse memories. By virtue of this combination, mols. and biol. particles, such as phage and viral particles and cells, that are in proximity or in phys. contact with the matrix combination can be labeled by programming the memory with identifying information and can be identified by retrieving the stored information. Combinations of matrix materials, memories, and linked mols. and biol. materials are also provided. The combinations have a multiplicity of applications, including combinatorial chem., isolation and purifn. of target macromols., capture and detection of macromols. for anal. purposes, selective removal of contaminants, enzymic catalysis, chem. modification and other uses.

ST remotely programmable matrixes memory; memory device program app array combinatorial phage library

IT Electromagnetic field
(as tags; remotely programmable matrixes with memories)

IT Chromatographs
(columns; remotely programmable matrixes with memories)

IT Containers
(contg. the matrixes with memories; remotely programmable matrixes with memories)

IT **Information systems**
(**data**; remotely programmable matrixes with memories)

IT Immunoassay
(immunoblotting; remotely programmable matrixes with memories)

IT Analytical apparatus
Antifuses
Combinatorial chemistry
Combinatorial library
Computer application
DNA microarray technology
Immobilization, molecular
Immunoassay
Memory devices
Microtiter plates
Northern blot hybridization
Nucleic acid hybridization
Optical detectors
Phage display library
Process automation
Solid phase synthesis
Southern blot hybridization
Test tubes
Vials
(remotely programmable matrixes with memories)

IT DNA
Proteins
RNA
RL: ANT (Analyte); CRT (Combinatorial reactant); RCT (Reactant); ANST (Analytical study); CMBI (Combinatorial study); RACT (Reactant or reagent)
(remotely programmable matrixes with memories)

IT 9004-70-0, Nitrocellulose
RL: DEV (Device component use); USES (Uses)
(remotely programmable matrixes with memories)

RE.CNT 62 THERE ARE 62 CITED REFERENCES AVAILABLE FOR THIS RECORD

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L43 ANSWER 16 OF 16 HCAPLUS COPYRIGHT 2003 ACS
AN **2001:916365** HCAPLUS
DN **136:34255**
TI Remotely programmable matrices with memories
IN Nova, Michael P.; Senyei, Andrew E.; David, Gary S.
PA Discovery Partners International, USA
SO U.S., 35 pp., Cont.-in-part of U.S. Ser. No. 428,662.

CODEN: UCXXAM
DT Patent
LA English
IC ICM G01N015-06
ICS G01N033-53; C12Q001-68; A61K038-00
NCL 422/68.1
CC **9-1 (Biochemical Methods)**
Section cross-reference(s): 7, 80
FAN.CNT 70

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 6331273	B1	20011218	US 1995-473660	19950607
	US 5741462	A	19980421	US 1995-427662	19950425
	US 5985562	A	19990720	US 1995-460196	19950607
	US 5874214	A	19990223	US 1995-538367	19951003
	US 6025129	A	20000215	US 1995-567746	19951205
	CA 2216645	AA	19961031	CA 1996-2216645	19960425
	WO 9636436	A1	19961121	WO 1996-US6145	19960425
	W: AL, AM, AT, AU, AZ, BB, BG, BR, BY, CA, CH, CN, CU, DE, DK, EE, ES, FI, GB, GE, HU, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI				
	RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN				
	EP 820361	A1	19980211	EP 1996-916437	19960425
	F: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI				
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	JP 11511338	T2	19990928	JP 1996-530562	19960425
	AU 9659285	A1	19961129	AU 1996-59285	19960501
	AU 707444	B2	19990708		
	US 6100026	A	20000808	US 1996-638410	19960610
	US 6319668	B1	20011120	US 1996-669052	19960624
	US 6264459	B1	20010904	US 1996-711426	19960905
	US 6017496	A	20000125	US 1996-709433	19960906
	US 5961923	A	19991005	US 1996-723423	19960930
	US 6329139	B1	20011211	US 1997-917998	19970811
	US 6340565	B1	20020122	US 1998-51002	19980402
PRAI	US 1995-428662	A2	19950425		
	US 1995-460196	A	19950607		
	US 1995-484504	A2	19950607		
	US 1995-473660	A	19950607		
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	US 1995-484504	A2	19950607		
	US 1995-538367	A2	19951003		
	US 1995-567746	A	19951205		
	US 1996-639813	A	19960402		
	WO 1996-US6145	W	19960425		
	US 1996-638410	A2	19960610		
	US 1996-669052	A2	19960624		
	US 1996-711426	A2	19960905		
	US 1996-709433	A2	19960906		
	US 1996-723423	A2	19960930		
	WO 1996-US15099	A2	19961003		
	US 1996-726703	B2	19961007		
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	US 1996-741685	B2	19961031		
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AB The invention concerns combinations, called matrixes with memories, of matrix materials with remotely addressable or remotely programmable

recording devices that contain at least one data storage unit are provided. The matrix materials are those that are used in as supports in solid phase chem. and biochem. syntheses, immunoassays and hybridization reactions. The data storage units are preferably non-volatile antifuse memories. By virtue of this combination, mols. and biol. particles, such as phage and viral particles and cells, that are in proximity or in phys. contact with the matrix combination can be labeled by programming the memory with identifying information and can be identified by retrieving the stored information. Combinations of matrix materials, memories, and linked mols. and biol. materials are also provided. The combinations have a multiplicity of applications, including combinatorial chem., isolation and purifn. of target macromols., capture and detection of macromols. for anal. purposes, selective removal of contaminants, enzymic catalysis, chem. modification and other uses. Methods for electronically tagging mols. are biol. particles and matrix support materials and immunoassays and other methods are also provided. Diagrams describing the app. are given.

ST memory device program app array combinatorial phage library

IT Electromagnetic field
(as tags; remotely programmable matrixes with memories)

IT Chromatographs
(columns; remotely programmable matrixes with memories)

IT Containers
(contg. the matrixes with memories; remotely programmable matrixes with memories)

IT **Information systems**
(**data**; remotely programmable matrixes with memories)

IT Immunoassay
(immunoblotting; remotely programmable matrixes with memories)

IT Analytical apparatus
Antifuses
Combinatorial chemistry
Combinatorial library
Computer application
DNA microarray technology
Immobilization, molecular
Immunoassay
Memory devices
Microtiter plates
Northern blot hybridization
Nucleic acid hybridization
Optical detectors
Phage display library
Process automation
Solid phase synthesis
Southern blot hybridization
Test tubes
Vials
(remotely programmable matrixes with memories)

IT DNA
Proteins
RNA
RL: ANT (Analyte); CFT (Combinatorial reactant); RCT (Reactant); ANST (Analytical study); CMBI (Combinatorial study); RACT (Reactant or reagent)
(remotely programmable matrixes with memories)

IT 9004-70-0, Nitrocellulose
RL: DEV (Device component use); USES (Uses)
(remotely programmable matrixes with memories)

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L43 ANSWER 11 OF 16 HCAPLUS COPYRIGHT 2003 ACS
AN 2001:397174 HCAPLUS
DN 134:363648
TI Method, apparatus, media and **signals** for identifying associated cell **signaling proteins**
IN **Pelech, Steven**
PA The University of British Columbia, Can.
SO PCT Int. Appl., 90 pp.
CODEN: PIXXD2
DT **Patent**
LA English
IC ICM G01N033-68
CC **9-1 (Biochemical Methods)**
FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2001033679	A2	20010531	WO 2000-CA1378	20001117
	W: AU, CA, JP, NZ, US				

PW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR
EP 1134287 A2 20020828 EP 2000-979297 20001117
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI, CY, TR
PRAI CA 1999-2290335 A 19991119
CA 1999-2290204 A 19991122
US 2000-216357P P 20000705
WO 2000-CA1378 W 20001117

AB Methods, app., media and **signals** for identifying assocd. cell **signaling proteins** are disclosed. The method involves producing and storing a comparison value for each pair of the cell **signaling proteins** in response to data values representing phys. properties of resp. cell **signaling proteins**. The method further involves identifying cell **signaling protein** pairs having comparison values satisfying a condition indicative of an assocn. between the cell **signaling proteins**.

ST app media **signal** identifying cell **signaling protein**

IT **Memory devices**
(**RAM** (**random access**); method, app., media and **signals** for identifying assocd. cell **signaling proteins**)

IT **Information systems**
(**data**; method, app., media and **signals** for identifying assocd. cell **signaling proteins**)

IT Gene
(expression, co-; method, app., media and **signals** for identifying assocd. cell **signaling proteins**)

IT Apparatus
Cell
Gel electrophoresis
Memory devices
Physical properties
Polyacrylamide gel electrophoresis
Signal transduction, biological
(method, app., media and **signals** for identifying assocd. cell **signaling proteins**)

IT Phosphorylation, biological
(**protein**; method, app., media and **signals** for identifying assocd. cell **signaling proteins**)

IT **Proteins**, specific or class
RL: ANT (Analyte); ANST (Analytical study)
(**signaling**, cee; method, app., media and **signals** for identifying assocd. cell **signaling proteins**)

IT **Information systems**
(**storage**; method, app., media and **signals** for identifying assocd. cell **signaling proteins**)

L43 ANSWER 12 OF 16 HCAPLUS COPYRIGHT 2003 ACS
AN 2001:397172 HCAPLUS
DN 135:2565
TI Multiblot kinase analysis
IN **Pelech, Steven**
PA The University of British Columbia, Can.
SO PCT Int. Appl., 61 pp.
CODEN: PIXXD2
DT **Patent**
LA English
IC ICM G01N033-573
CC 9-16 (Biochemical Methods)
Section cross-reference(s): 7

FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2001038877	A2	20010531	WO 2000-CA1377	20001117
	W: AU, CA, JP, NZ, US				
	RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR				
	EP 1234184	A2	20020828	EP 2000-979296	20001117
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI, CY, TR				
PRAI	CA 1999-2290335	A	19991119		
	CA 1999-2290204	A	19991122		
	US 2000-216357P	P	20000705		
	WO 2000-CA1377	W	20001117		

AB This invention provides a method for detection of multiple kinases or multiple kinase substrates, whereby the presence and phosphorylation state of a large no. kinases and/or kinase substrate proteins may be tracked in a single sample electrophoretically sepg. in one dimension, proteins in a sample to be tested for kinase or kinase substrate content; to produce an array of proteins so sepd. contacting the array with two or more antibodies selected from anti-kinase and anti-kinase substrate antibodies; and, detecting the presence of said antibodies bound to kinases or kinase substrate moieties in the array. This method may also comprise recording one or more values representative of a location for each of said detected antibodies bound to proteins in the array indicative of a location of a kinase or kinase substrate in the array.

ST multiblot kinase analysis

IT **Information systems**
(**data**; multiblot kinase anal.)

IT Immunoassay
(immunoblotting; multiblot kinase anal.)

IT Electrophoresis
Membranes, nonbiological
Mixtures
Photographic films
Polyacrylamide gel electrophoresis
Recording
Samples
(multiblot kinase anal.)

IT Proteins, general, analysis
RL: ANT (Analyte); ANST (Analytical study)
(multiblot kinase anal.)

IT Antibodies
RL: ARG (Analytical reagent use); ANST (Analytical study); USES (Uses)
(multiblot kinase anal.)

IT Phosphorylation, biological
(protein; multiblot kinase anal.)

IT **Information systems**
(**storage**; multiblot kinase anal.)

IT 9031-44-1, Kinase (phosphorylating)
RL: ANT (Analyte); ANST (Analytical study)
(multiblot kinase anal.)

IT 56-65-5, 5'-ATP, uses
RL: ARG (Analytical reagent use); ANST (Analytical study); USES (Uses)
(multiblot kinase anal.)

IT 9025-75-6, Phosphoprotein phosphatase
RL: ARU (Analytical role, unclassified); CAT (Catalyst use); ANST (Analytical study); USES (Uses)
(multiblot kinase anal.)

IT 79-06-1, Acrylamide, uses 110-26-9, Bisacrylamide
RL: NUU (Other use, unclassified); USES (Uses)
(multiblot kinase anal.)

L43 ANSWER 13 OF 16 HCAPLUS COPYRIGHT 2003 ACS
AN **2000:551303** HCAPLUS
DN **133:161561**
TI Apparatus for supporting **protein** analysis, and memory medium accommodating program for computer treatment with this apparatus
IN Kitajima, Masato; Oya, Michihiro
PA Fujitsu Ltd., Japan
SO Jpn. Kokai Tokkyo Koho, 10 pp.
CODEN: JKXXAF
DT Patent
LA Japanese
IC ICM G06F017-30
ICS G01N033-48; G01N033-566
CC **9-1** (**Biochemical Methods**)
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI JP 2000222421	A2	20000811	JP 1999-23997	19990129
JP 3370942	B2	20030127		
PRAI JP 1999-23997		19990129		

AB An app. for supporting **protein** anal. is designed so that the amino acid residue parts of a **protein** interacting with a low mol. wt. compd. are extd. in the form contg. the max. quantity of information on the structure of the **protein**. Using information from database (e.g., **Protein** Data Bank(PDB)), the amino acid residues contg. a specified kind of atom in the specified **protein** present within a certain distance from a resp. specified kind fo atom in the specified compd. are searched. Then, a sequence pattern is formed by putting each amino acid residue obtained as a result of the search according to the certain notation rule in the order of the primary sequence of amino acid residues constituting the specified **protein** . This sequence pattern is made available as the information expressing the primary sequence structure at the part of the **protein** contg. the amino acid residue part interacting with the specified compd. A flow chart describing the treatment procedures for forming motif pattern is given.
ST **protein** analysis amino acid sequence database
IT Apparatus
Computer program
Databases
Memory devices
Nomenclature, general
Protein sequences
(app. for supporting **protein** anal., and memory medium accommodating program for computer treatment with app.)
IT **Proteins**, general, biological studies
RL: BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)
(app. for supporting **protein** anal., and memory medium accommodating program for computer treatment with app.)
IT **Information systems**
(**data**; app. for supporting **protein** anal., and memory medium accommodating program for computer treatment with app.)
IT Amino acids, biological studies
RL: BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)
(residues; app. for supporting **protein** anal., and memory medium accommodating program for computer treatment with app.)

L43 ANSWER 14 OF 16 HCAPLUS COPYRIGHT 2003 ACS
AN 1999:176020 HCAPLUS
DN 132:206134
TI Method for the rapid screening of drug candidates or other analytes

IN Pauwels, Rudi Wilfried Jan; Roelant, Christiaan Hubert Simon; Van Acker, Koenraad Lodewijk August

PA Tibotec N.V., Belg.

SO PCT Int. Appl., 63 pp.
CODEN: PIXXD2

DT Patent

LA English.

IC ICM G01N033-543
ICS B01L003-02; G01N033-569; G01N033-573; C12Q001-18

CC 1-1 (Pharmacology)
Section cross-reference(s): **3**, **9**, 15

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2000014540	A1	20000316	WO 1998-IB1369	19980908
	W: AU, BR, CA, CN, IL, JP, KR, MX, NZ, PL, RU, SG, TR, US				
	RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
	CA 2341627	AA	20000316	CA 1998-2341627	19980908
	AU 2000022512	A5	20000327	AU 2000-22512	19980908
	BR 9816009	A	20010605	BR 1998-16009	19980908
	EP 1114494	A1	20010704	EP 1998-940489	19980908
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, FI				
	EP 1250955	A1	20021023	EP 2001-204142	19980908
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, FI, CY				
	JP 2003517575	T2	20030527	JP 2000-569264	19980908
	TW 439312	B	20010411	TW 2000-89104946	20000221
	ZA 2000000891	A	20000913	ZA 2000-891	20000223
	US 2002081629	A1	20020627	US 2001-25391	20011219
PRAI	EP 1998-940489	A3	19980908		
	WO 1998-IB1369	A	19980908		
	US 2000-530907	A3	20000630		

AB A method for the rapid screening of analytes, e.g. potential drug candidates, comprises the steps of applying a plurality of analytes to be screened onto one or more solid support(s) such that the analytes remain isolated from one another; contacting the analyte-carrying solid support(s) with targets provided in a semi-solid or liq. medium, whereby the analytes are released from the solid support(s) to the targets; and measuring analyte-target interactions. This method allows for the manipulation of thousands of different analytes simultaneously. When the analyte is applied to the solid support, it can diffuse thereon so as to produce a concn. gradient and serial diln. of analyte if a dose response curve for a candidate drug is required. The method described can be readily automated.

ST drug analyte screening method app; automated drug analyte screening method app

IT Animal cell line
(MT-4; rapid screening method for drug candidates or other analytes)

IT Liposomes
(and beads; rapid screening method for drug candidates or other analytes)

IT Analysis
Analysis
Process automation
Process automation
(automated anal.; rapid screening method for drug candidates or other analytes)

IT Eukaryote (Eukaryotae)
Prokaryote
(cell; rapid screening method for drug candidates or other analytes)

IT **Information systems**
(electronic or magnetic or digitized; rapid screening method for drug

candidates or other analytes)
IT **Proteins**, specific or class
FL: BPP (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(green fluorescent; rapid screening method for drug candidates or other analytes)
IT Pens
(including plotter pens; rapid screening method for drug candidates or other analytes)
IT Spectroscopy
(luminometry; rapid screening method for drug candidates or other analytes)
IT Monolayers
(mol. or cellular; rapid screening method for drug candidates or other analytes)
IT Containers
(print head; rapid screening method for drug candidates or other analytes)
IT Analysis
Analytical apparatus
Antiviral agents
Capillary tubes
Cell
Ceramics
Charge coupled devices
Colorimetry
Containers
Conveyor belts
Densitometry (optical)
Diffusion
Drug screening
Films
Fluorescence microscopy
Fluorometry
Human immunodeficiency virus 1
Immobilization, biochemical
Langmuir-Blodgett films
Membranes, nonbiological
Microscopy
Microtiter plates
Molecules
Optical ROM disks
Photographic films
Physical properties
Radiochemical analysis
Sensors
Smart materials
Virus
(rapid screening method for drug candidates or other analytes)
IT Antibodies
Antigens
Probes (nucleic acid)
FL: ANT (Analyte); ANST (Analytical study)
(rapid screening method for drug candidates or other analytes)
IT Gelatins, uses
FL: DEV (Device component use); USES (Uses)
(rapid screening method for drug candidates or other analytes)
IT Glass, uses
FL: DEV (Device component use); USES (Uses)
(rapid screening method for drug candidates or other analytes)
IT Metals, uses
FL: DEV (Device component use); USES (Uses)
(rapid screening method for drug candidates or other analytes)

IT Polymers, uses
PL: DEV (Device component use); USES (Uses)
(rapid screening method for drug candidates or other analytes)
IT Polysaccharides, uses
PL: DEV (Device component use); USES (Uses)
(rapid screening method for drug candidates or other analytes)
IT Materials
(tapes; rapid screening method for drug candidates or other analytes)
IT Receptors
PL: PPR (Biological process); BSU (Biological study, unclassified); PEP (Physical, engineering or chemical process); BIOL (Biological study); PROC (Process)
(target; rapid screening method for drug candidates or other analytes)
IT Containers
(tubes; rapid screening method for drug candidates or other analytes)
IT 9068-38-6, Reverse transcriptase
PL: BSU (Biological study, unclassified); BIOL (Biological study)
(inhibitors; rapid screening method for drug candidates or other analytes)
IT 1461-15-0, Calcein
PL: ARG (Analytical reagent use); ANST (Analytical study); USES (Uses)
(rapid screening method for drug candidates or other analytes)
IT 80516-87-1, AZT 134678-17-4, 3TC 147362-17-0, Loviride
PL: PAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(rapid screening method for drug candidates or other analytes)
IT 9002-18-0, Agar 9003-05-8, Polyacrylamide 9003-53-6, Polystyrene 9004-34-6, Cellulose, uses 9004-67-5, Methylcellulose 9012-36-6, Agarose
PL: DEV (Device component use); USES (Uses)
(rapid screening method for drug candidates or other analytes)
IT 7631-86-9, Silicon dioxide, uses
PL: DEV (Device component use); USES (Uses)
(wafer; rapid screening method for drug candidates or other analytes)
RE.CNT 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD
RE
(1) Andres, B; WO 9711571 A 1998 HCAPLUS
(2) Burstein Lab Inc; WO 9801533 A 1998 HCAPLUS
(3) Du Pont; GB 2008767 A 1979 HCAPLUS
(4) Ekins, R; ANNALES DE BIOLOGIE CLINIQUE 1992, V50(5), P337 HCAPLUS
(5) Leaback, D; US 4276048 A 1981 HCAPLUS
(6) Pharmacopeia Inc; WO 9716569 A 1997 HCAPLUS
(7) Sigal, N; COMB CHEM MOL DIVERSITY DRUG DISCOVERY P433

L43 ANSWER 15 OF 16 HCAPLUS COPYRIGHT 2003 ACS
AN **1989:456544** HCAPLUS
DN **111:56544**
TI An electronic database for molecular biology
AU Burridge, Jane M.
CS IBM, Winchester/Hants., SO23 8BY, UK
SO Biochemical Society Transactions (1989), 17(5), 840-1
CODEN: BCSTB5; ISSN: 0300-5127
DT Journal
LA English
CC 20-5 (History, Education, and Documentation)
Section cross-reference(s): 6
AB The development of a compact disk-read only memory (CD-ROM) mol. database is described which will make numerical data, text, graphics, and images available to be browsed, searched, and manipulated interactively. The CD-ROM publication will hold numerical data defining 400 or so large **protein** mols. together with several hundred high-resoln. color pictures depicting these mols., several key texts describing properties,

regularities, and peculiarities of the mols., and some programs.
ST **protein** compact disk format database
IT **Proteins**, uses and miscellaneous
PL: USES (Uses)
(database of, compact disk-read only memory format of, development of)
IT **Memory devices**
(**optical, disks, read-only,**
protein database on format of, development of)
IT **Information science and technology**
(**system, computerized,** of **proteins,**
compact disk-read only memory format of, development of)

L43 ANSWER 16 OF 16 HCAPLUS COPYRIGHT 2003 ACS
AN **1987:570984** HCAPLUS
DN **107:170984**
TI A DNA and **protein** database system on CD-ROM
AU Nasu, Hisanori; Itoh, Toshiaki
CS Hitachi Software Eng. Co., Ltd., Yokohama, 231, Japan
SO Joho Kanri (1986), 29(8), 657-66
CODEN: JOKAAB; ISSN: 0021-7298
DT Journal
LA Japanese
CC 6-7 (General Biochemistry)
Section cross-reference(s): 3, 10
AB DNASIS-DBFEF31 is an information storage and retrieval system for DNA and **protein** ref. and sequence data. The data and software are loaded on CD-ROM. The system can be run on Hitachi B-16, NEC PC 9801 series or IBM PC-XT/AT personal computers. The source files of the database are GenBank, EMBL, and NBRF. The system has capabilities for retrieval of ref. information as well as homol. searching for sequence data.
ST CD ROM DNA **protein** sequence database
IT Deoxyribonucleic acid sequences
Protein sequences
(database of, on CD-ROM)
IT **Memory devices**
(**optical, disks, read-only,** DNA
and **protein** databases on)
IT **Information science and technology**
(**system, computerized,** for DNA and **protein**
sequences, on CD-ROM)

=> d all tot

L47 ANSWER 1 OF 6 HCAPLUS COPYRIGHT 2003 ACS
AN 2002:869628 HCAPLUS
DN 137:334941
TI Analysis mechanism for genetic data
IN Hytopoulos, Evangelos; Miller, Brett; Ray, Sandip
PA X-Mine, USA
SO U.S. Pat. Appl. Publ., 34 pp.
CODEN: USXXCO
DT Patent
LA English
IC ICM G06F019-00
ICS G01N033-48; G01N033-50
NCL 702019000
CC **9-16** (**Biochemical Methods**)
Section cross-reference(s): 3
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 2002160560	A1	20021114	US 2001-854427	20010512

PRAI US 2001-854427 20010512
AB Results of statistical **clustering** and/or correlation anal. of genetic or proteomic expression data such as microarrays, gene chips, or **protein** chips are used, e.g., as response variables, in further anal. of expression data. In particular, an array of expression data is **clustered** using a **cluster** tool to produce an array of expression **clusters**. Each of the expression **clusters** represents the same expts. represented by the original expression array. Accordingly, each **cluster** of the array is of the proper form to be used as a response variable of expression values. Using an expression **cluster** as a response variable for either supervising **clustering** or correlation anal. allows correlation between such an expression **cluster** and other expression data.
ST analysis mechanism genetics
IT **Cluster analysis**
Computer application
Computers
Configuration
Correlation analysis
DNA microarray technology
Gene expression profiles
Genetics
Memory devices
Microarray technology
Protein microarray technology
(anal. mechanism for genetic data)
IT Gene
Proteins
Proteome
PL: ANT (Analyte); BSU (Biological study, unclassified); ANST (Analytical study); BIOL (Biological study)
(anal. mechanism for genetic data)
IT **Information systems**
(**data**; anal. mechanism for genetic **data**)
IT Education
(instructions; anal. mechanism for genetic data)

L47 ANSWER 3 OF 6 HCAPLUS COPYRIGHT 2003 ACS
AN 2002:450025 HCAPLUS
DN 137:16492
TI Computer-based **cluster** analysis of gene expression patterns
IN Kobayashi, Takeshi; Honda, Hiroyuki; Hanai, Taizou; Tomita, Shuta
PA Nagoya Industrial Science Research Institute, Japan
SO PCT Int. Appl., 134 pp.
CODEN: PIXXD2
DT Patent
LA Japanese
IC ICM G06F017-30
ICS C12N015-00
CC 3-1 (Biochemical Genetics)
Section cross-reference(s): **9**, 20
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 2002046962	A1	20020613	WO 2001-JP10704	20011206

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR,

PF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MP, NE, SN, TD, TG

JP 2002175306 A2 20020621 JP 2000-377765 20001208
AU 2002031076 A5 20020618 AU 2002-31076 20011206
PRAI JP 2000-377765 A 20001208
WO 2001-JP10704 W 20011206

AB A method and app. for **clustering** anal. of data for gene expression patterns using computer programs and computer readable memory storage device, are disclosed. Genes are **clustered** by acquiring **signal** patterns showing the expression states of the genes and then processing the **signal** patterns thus acquired by using the ART technique. Examn. of gene expression patterns in Saccharomyces cerevisiae wild type using Fuzzy ART program is described. Data are displayed in groups.

ST gene expression **cluster** analysis computer program

IT **Computer program**
(ART, Fuzzy ART; computer-based **cluster** anal. of gene expression patterns)

IT **Bioinformatics**
Cluster analysis
Computer application
Computers
Magnetic memory devices
(computer-based **cluster** anal. of gene expression patterns)

IT Gene
RL: ANT (Analyte); BSU (Biological study, unclassified); ANST (Analytical study); BIOL (Biological study)
(expression; computer-based **cluster** anal. of gene expression patterns)

RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD

RE
(1) Frank, T; IEEE TRANSACTIONS ON NEURAL NETWORKS 1998, V9(3), P544
(2) Hirashi, A; Nippon Biseibutsu Seitai Gakkaiho 1999, V10(3), P119
(3) Tsujimoto, G; Chapter 2: Transcript-.mu.m Kaiseki; IV Bio Informatics; 1 Transcript-.mu.m Informatics 2000, P121

L47 ANSWER 3 OF 6 HCAPLUS COPYRIGHT 2003 ACS
AN 2002:241116 HCAPLUS
DN 136:258302
TI Phylogenetic tree diagram display for gene expression data **cluster** analysis
IN Nozaki, Yasuyuki; Nakashige, Eyo; Tamura, Takuri
PA Hitachi Software Engineering Co., Ltd., Japan
SO PCT Int. Appl., 49 pp.
CODEN: PIXXD2
DT Patent
LA Japanese
IC ICM G06F017-30
ICS G06F019-00; G01N033-50; C12N015-11
CC 9-1 (Biochemical Genetics)
Section cross-reference(s): **9**, 30

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2002025489	A1	20020328	WO 2000-JP6385	20000919
	W: JP, US				
	RW: DE, FR, GB				
PRAI	WO 2000-JP6385		20000919		

AB A system of **cluster** anal. for gene expression data from DNA microarray hybridization is described that uses std. statistical algorithms to arrange genes according to similarity in pattern of gene expression. The output is displayed graphically, in the form of phylogenetic tree diagram, conveying the **clustering** and the underlying expression data simultaneously in a form intuitive for

biologists. A threshold indicating a similarity of expression patters is preset, and genes with the same function and genes similar in expression pattern to those genes are extd. and displayed. In addn., an expt. pattern required by **clustering** is reselected for the extd. genes and is then used to subject them to **cluster** anal. How many individual functions are available in genes belonging to a partial tree is calcd. to det. ratio in which individual functions account for in a partial tree. If their ratios in the partial tree exceed the preset threshold, they are regarded as a **cluster** (set of genes similar in function) and are subjected to extn. processing.

ST evolution tree diagram computer graphic display genetics **cluster** analysis; **cluster** analysis genome expression DNA microarray hybridization

IT Audiovisual aids
(diagrams; phylogenetic tree diagram display for gene expression data **cluster** anal.)

IT Gene
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(expression; phylogenetic tree diagram display for gene expression data **cluster** anal.)

IT Evolution
(mol.; phylogenetic tree diagram display for gene expression data **cluster** anal.)

IT **Bioinformatics**
Cluster analysis
Computer application
Computer program
DNA microarray technology
Information, biological
Magnetic memory devices
(phylogenetic tree diagram display for gene expression data **cluster** anal.)

RE.CNT 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD

RE

(1) Fujitsu Limited; JP 07-274965 A 1997
(2) Fujitsu Limited; GB 2313840 A 1997
(3) Fujitsu Limited; US 5598350 A 1997
(4) Foss, D; Nature Genetics 2000, V24(3), P227 HCAPLUS

L47 ANSWER 4 OF 6 HCAPLUS COPYRIGHT 2003 ACS
AN 2001:741258 HCAPLUS
DN 135:283937
TI Computer-based **cluster** analysis and display of gene expression patterns
IN Nakashige, Akira; Nozaki, Yasuyuki; Watanabe, Tsunehiko; Tamura, Takao
PA Hitachi Software Engineering Co., Ltd., Japan
SO Jpn. Kokai Tokkyo Koho, 10 pp.
CODEN: JKXXAF
DT Patent
LA Japanese
IC ICM G01N033-53
ICS C12M001-00; G01N033-566; G01N035-00; G01N035-02; G01N037-00; G16B015-00
CC 6-1 (Biochemical Genetics)
Section cross-reference(s): **9**, 20

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 2001281244	A2	20011010	JP 2000-88695	20000328
PRAI	JP 2000-88695		20000328		

AB A method and materials for graphic display of data on gene expression patterns obtained via **clustering** anal. using computer programs and computer readable memory storage device, are disclosed. Data are

displayed in groups.
ST gene expression **cluster** analysis computer program graphic display
IT **Bioinformatics**
Cluster analysis
Computer application
Computer program
Computers
Magnetic memory devices
(computer-based **cluster** anal. and display of gene expression patterns)
IT Gene
(expression; computer-based **cluster** anal. and display of gene expression patterns)

L47 ANSWER 5 OF 6 HCAPLUS COPYRIGHT 2002 ACS
AN 2001:507491 HCAPLUS
DN 135:69544
TI Database system and method useful for predicting putative ligand binding sites
IN Edelman, Marvin; Kuttner, Yosef; Sobolev, Vladimir
PA Yeda Research and Development Co. Ltd., Israel
SO PCT Int. Appl., 49 pp.
CODEN: PIXXD2
DT Patent
LA English
IC ICM A61K
CC **9-16** (**Biochemical Methods**)
Section cross-reference(s): 6, 7, 20

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2001049244	A2	20010712	WO 2001-IL9	20010102
	WO 2001049244	A3	20020307		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

PRAI IL 2000-133866 A 20000103
AB A method of identifying at least one consensus structural characteristic of binding sites of a ligand of interest is provided. The method is effected by: (a) obtaining structural data pertaining to a plurality of **proteins** while complexed with the ligand of interest; and (b) extg. from the structural data at least one consensus structural characteristic characterizing an interaction between the ligand of interest and at least one of the plurality of **proteins**, thereby identifying at least one consensus structural characteristic of binding sites of the ligand of interest. The process for identification of a consensus structural characteristic of binding sites for ATP is described. A non-redundant dataset of **protein**/ANP complexes was prepd. and used.
ST database system predicting ligand binding site **protein** structure; ATP binding site **protein** consensus structure
IT **Algorithm**
(**CLUSTER**; database system and method useful for predicting putative ligand binding sites)
IT Heat-shock **proteins**
RL: BPR (Biological process); BSU (Biological study, unclassified); PRP

(Properties); BIOL (Biological study); PROC (Process)
(HSP 70, 44-kD N-terminal fragment, as ATP-binding **protein**; database system and method useful for predicting putative ligand binding sites)

IT Insulin receptors
Myosins
RL: BPR (Biological process); BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study); PROC (Process)
(as ATP-binding **proteins**; database system and method useful for predicting putative ligand binding sites)

IT **Optical disks**
(computer; database system and method useful for predicting putative ligand binding sites)

IT **Information systems**
(**data**; database system and method useful for predicting putative ligand binding sites)

IT **Proteins**, general, properties
RL: PEP (Properties)
(database PDB; database system and method useful for predicting putative ligand binding sites)

IT Apparatus
Cluster analysis
Computer program
Computers
Data processing
Databases
Magnetic memory devices
Optical memory devices
(database system and method useful for predicting putative ligand binding sites)

IT Ligands
RL: BPR (Biological process); BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study); PROC (Process)
(database system and method useful for predicting putative ligand binding sites)

IT **Optical disks**
(digital video disk (DVD); database system and method useful for predicting putative ligand binding sites)

IT Structure-activity relationship
(ligand-binding; database system and method useful for predicting putative ligand binding sites)

IT **Proteins**, specific or class
RL: BPR (Biological process); BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study); PROC (Process)
(ligand-binding; database system and method useful for predicting putative ligand binding sites)

IT **Magnetic disks**
Optical disks
(magnetooptical disks; database system and method useful for predicting putative ligand binding sites)

IT **Information systems**
(**network**; database system and method useful for predicting putative ligand binding sites)

IT Actins
RL: BPR (Biological process); BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study); PROC (Process)
(profilactins, .beta.-actin, as ATP-binding **proteins**; database system and method useful for predicting putative ligand binding sites)

IT **Information systems**
(**storage**; database system and method useful for predicting putative ligand binding sites)

IT Actins

RL: BPR (Biological process); BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study); PROC (Process)
(.beta.-, complexes with profilin, as ATP-binding **proteins**; database system and method useful for predicting putative ligand binding sites)

IT 52660-18-1
RL: BPR (Biological process); BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study); PROC (Process)
(3 .alpha.-subunit or 1, as ATP-binding **protein**; database system and method useful for predicting putative ligand binding sites)

IT 9001-83-6, Phosphoglycerate kinase 9001-89-2, Phosphorylase kinase 9013-49-1, Aspartate transcarbamylase 9013-02-9, Adenylate kinase 9032-64-3, NAD synthetase 9073-94-3, Phosphoenolpyruvate carboxykinase 141349-86-2, cyclin-dependent kinase 2 142018-29-3, CAMP-dependent **protein** kinase 145529-86-2, Hematopoietic cellular kinase
RL: BPR (Biological process); BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study); PROC (Process)
(as ATP-binding **protein**; database system and method useful for predicting putative ligand binding sites)

IT 56-65-5, ATP, biological studies 56-65-5D, ATP, analogs, biological studies
RL: BPR (Biological process); BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study); PROC (Process)
(as ligand; database system and method useful for predicting putative ligand binding sites)

IT 25612-73-1
RL: BPR (Biological process); BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study); PROC (Process)
(database system and method useful for predicting putative ligand binding sites)

L47 ANSWER 6 OF 6 HCAPLUS COPYRIGHT 2003 ACS
AN 1993:471898 HCAPLUS
DN 119:71898
TI Substructure searching on very large files by using multiple storage techniques
AU Bartmann, Alexander; Maier, Helmut; Walkowiak, Dirk; Roth, Bernard; Hicks, Martin G.
CS Softron GmbH, Graefelfing, D8032, Germany
SO Journal of Chemical Information and Computer Sciences (1993), 33(4), 539-41
CODEN: JCISD8; ISSN: 0095-2338
DT Journal
LA English
CC 20-5 (History, Education, and Documentation)
AB Traditional substructure search systems use a 2-stage algorithm consisting of a preliminary screening which operates on (inverted) index files to det. a set of candidates to be processed by the atom-by-atom search (ABAS). The screening stage is usually fast, the performance of the system being governed by the screening efficiency. If a large no. of candidates is left after the screening, the result is often a very large increase in retrieval time. The ABAS becomes the time-dependent stage due to the excessively large no. of disk seeks required to get the randomly distributed structure records into memory. The new search algorithm described in this paper is based on a special preprocessed structure file. It contains multiples of each mol.'s connection table organized in **clusters** forming contiguous portions of the search file. Each **cluster** can be characterized by a substructure contained in all its mols. A mol. may be a member of several different **clusters**, or it may appear repeatedly in the same **cluster**. File generation and update is fast and simple, and the mass storage requirements are only .apprx.1 kbyte/mol. A substructure search is performed by finding the min. set of **clusters** contg. all

candidates for a given query. The ABAS only has to scan sequentially through the relevant portions of the structure file. Furthermore, each single I/O-operation can read hundreds of structures into memory. Only the structures that are not already verified to be hits by the screening must be processed. The ABAS is CPU-bound. This architecture offers an extremely good performance on very large files for various computer platforms (e.g., IBM-PC, IBM-Mainframe, VAX) and even on slow storage devices like CD-ROMs.

ST storage technique searching mol substructure

IT **Algorithm**
(for mol. substructure searching on large files using multiple storage techniques)

IT **Memory devices**
(**optical, disks, read-only,**
mol. substructure storage on, searching of)

IT **Information science and technology**
(**searching, computerized,** of mol. substructures, in large files using multiple **storage** techniques)

IT **Information science and technology**
(**storage,** of mol. substructures, for online **searching**
)

IT **Information science and technology**
(**storage, computerized,** of mol. substructures, for online **searching**)

IT Molecular structure
(substructure, searching of, in large files using multiple storage techniques)

=> fil compuscie
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FILE LAST UPDATED: 18 DEC 2002 <20021218/UP>
FILE COVERS 1972 TO DATE.

=> d all

L63 ANSWER 1 OF 1 COMPUSCIENCE COPYRIGHT 2003 FIZ KARLSRUHE
AN 1982(4):PH3022 COMPUSCIENCE
TI Biophysical and biochemical information transfer in recognition.
AU Editor(s): Vassileva-Popova, J.G.; Jensen, E.V.
SO New York: Plenum Press. 1979. 892 p.
Conference: 2. International Colloquium on Physical and Chemical Information Transfer in Regulation of Reproduction and Ageing (PCITRRA), Varna (Bulgaria), 3-8 Oct 1977
ISBN: 0-306-40036-7
DT Book; Conference
CY United States
LA English
IP FIZKA
AB In this issue, physical and chemical aspects of biological recognition are discussed. Mathematical approaches, models and hypotheses for studying biological recognition are involved. Further, application of physical and chemical aspects of biorecognition in development and ageing are inclused. An extraordinarily varied set of topics is to be found between the covers of this volume which contains the proceedings of the Colloquium-hormone activity and hormone receptors, cyclic AMP, membranes, microtubules, adenylate cyclase, the quantum mechanics of biological molecules, enzyme specificity and kinetics, brain peptides and proteins, prolactin, circadian rhythms, oscillatory reactions, and even such unorthodox investigations as the study of magnetic field effects and the

search for light guides in biological systems. So wide a range of investigation also requires new tools, and one section of the book is devoted to a discussion of new kinds of instrumentation - rapid spectrophotometers, lasers, and stopped-flow techniques. (orig.)
CC *B04-* Memory structures
ST BIOPHYSICS; HORMONES; ENZYMES; KININS; RECEPTORS; SPECIFICITY; AGING; MUSCLES; CELL MEMBRANES; PERMEABILITY; LABELLING; AUTORADIOGRAPHY; REPRODUCTION; MEMORY DEVICES; NERVOUS SYSTEM

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MOST RECENT DERWENT UPDATE: 200333 <200333/DW>
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L90 ANSWER 1 OF 5 WPIX (C) 2003 THOMSON DERWENT
AN **2002-631531** [68] WPIX
DNN **N2002-499397** DNC **C2002-178497**
TI Analysis of amino acid sequences and average characteristic values with continuous analytic parameters, to forecast structure and function of proteins.
DC B04 D16 **S03 T01**
PA (FUFO-I) FURUTANI M; (MATS-I) MATSUOKA F; (TSUK-I) TSUKAHARA T
CYC 1
PI JP 2002215635 A 20020802 (200268)* 19p G06F017-30 <--
ADT JP 2002215635 A JP 2001-13859 20010122
PRAI JP 2001-13859 20010122
IC ICM **G06F017-30**
ICS **G01N033-68; G06F019-00**
ICA C12N015-09
AB JP2002215635 A UPAB: 20021022
NOVELTY - A distribution analysis of amino acid sequences for the forecast of structure and functions of a protein, is new.
DETAILED DESCRIPTION - A distribution analysis of amino acid sequences for the forecast of structure and functions of a protein by:
(a) calculation of amino acid species based on the predetermined parameters for the read plural amino acid sequences;
(b) drawing of an amino acid distribution pattern for the analyzed individual amino acids; and

(c) forecasting the structure and functions of the protein on the basis of amino acid distribution pattern, is new.

USE - The method is useful for the analysis of the amino acid sequence of a protein, to forecast its structure and function.

ADVANTAGE - The method provides an easily operable analysis of functions and structures of amino acid sequences with pattern recognition.

DESCRIPTION OF DRAWING(S) - The drawing shows a flow chart explaining the method.

11 an apparatus for the analysis of amino acid distribution
112 a procedure of input and selection
113 a procedure for the memory of amino acid sequence data
114 a procedure for the memory of parameters
115 reading of amino acid sequence
116 a procedure for counting amino acid species
117 a procedure for sorting the calculated values
118 a procedure for plotting the amino acid distribution pattern
119 amino acid distribution diagram
120 a procedure for calculation of each segment
121 a procedure for establishment of category
122 a procedure for plotting category distribution pattern
123 category distribution diagram

Dwg.1/15

FS CPI EPI
FA AB; GI; DCN
MC CPI: B11-C08F3; B11-C08G; D05-H09
EPI: **S03-E14H; T01-J; T01-J05B**
ABEX UPTX: 20021022
EXAMPLE - No suitable example given.

L90 ANSWER 2 OF 5 WPIX (C) 2003 THOMSON DERWENT
AN **2002-608539** [66] WPIX
CR 2002-667079 [71]
DNN **N2002-481830** DNC **C2002-172137**
TI Machine implemented method for deriving oligomer sequence from mass spectrum data, by providing predetermined set of mass/charge values for monomer sequences and determining abundance value for each monomer.
DC B04 D16 **S03 T01** V05
IN HALL, M P; PETESCH, P; SCHNEIDER, L V
PA (TARG-N) TARGET DISCOVERY INC
CYC 96
PI WO 2002061661 A2 20020808 (200266)* EN 151p G06F019-00 <--
RW: AT BE CH CY DE DK EA ES FI FR GB GH GM GR IE IT KE LS LU MC MW MZ NL OA PT SD SE SL SZ TR TZ UG ZW
W: AE AG AL AM AT AU AZ BA BB BG BR BY BZ CA CH CN CO CR CU CZ DE DK DM DZ EC EE ES FI GB GD GE GH GM HR HU ID IL IN IS JP KE KG KP KR KZ LC LK LR LS LT LU LV MA MD MG MK MN MW MX MZ NO NZ PH PL PT RO RU SD SE SG SI SK SL TJ TM TR TT TZ UA UG UZ VN YU ZA ZW
ADT WO 2002061661 A2 WO 2001-US49491 20011019
PRAI US 2000-242398P 20001019; US 2000-242165P 20001019
IC ICM **G06F019-00**
ICS G16B001-00; **G01N033-68**; H01J049-00
AB WO 200261661 A UPAB: 20021108
NOVELTY - A machine implemented method (M1) for deriving sequence of a portion of oligomer from mass spectrum data (MSD), comprising providing predetermined set (PDS) of mass/charge (m/z) values for monomer sequences (MS), determining abundance value from MSD for each m/z value in PDS, thus producing number of abundance values, calculating a first ranking, for each sequence of set of MS having first number of monomer.

DETAILED DESCRIPTION - A machine implemented method for deriving a sequence of a portion of oligomer from mass spectrum data (MSD), comprising:

(a) providing predetermined set of mass/charge (m/z) values for monomer sequences each of which comprises a mass label;

(b) determining abundance value from MSD for each m/z value in the predetermined set, thus producing number of abundance values; and

(c) calculating a first ranking, based on abundance values, for each sequence of a set of monomer sequences having a first number of monomer.

INDEPENDENT CLAIMS are also included for the following:

(1) a machine readable medium containing executable computer program instructions, which when executed by a processing system cause the processing system to perform M1;

(2) processing (M2) noise in a mass spectrum data of a fragmented oligomer, comprising:

(a) determining a periodic block of noise in a mass spectrum data generated from accelerating fragments of an oligomer to a detector; and

(b) filtering the periodic block of noise from the mass spectrum data;

(3) determining (M3) a sequence of at least a portion of an oligomer from MSD, comprising:

(a) reading MSD in a first reading operation from a non-volatile storage device to a temporary volatile cache memory to obtain abundance values at a set of possible m/z values from the temporary volatile cache memory;

(b) calculating first abundance parameters from the abundance values, reading MSD in a second reading operation, following the first reading operation, from the temporary volatile cache memory to obtain the abundance values of the set of m/z values; and

(c) determining a ranking based on abundance values for each sequence of a set of monomer sequences having a first number of monomers; and

(4) processing (M4) MSD of extract specific labeled ions of interest, comprising determining a periodic block of noise in MSD generated from accelerating unlabeled ions to a detector and filtering the periodic block of noise from MSD.

USE - M1 is useful for deriving sequence of a portion of oligomer from MSD, where the oligomer is a protein, nucleic acid or oligosaccharide (claimed).

ADVANTAGE - M1 has the ability to sequence full proteins and nucleic acids without the need for prior digestion into small peptides or nucleic acids. The method is self-starting and does not require any knowledge of the parent ion size or composition to determine the sequence. The method has the ability to determine partial protein sequences from regions of a protein that may not contain ionizable amino acid residues.

Dwg.0/0

FS CPI EPI

FA AB; DCN

MC CPI: B04-C01; B04-C02X; B04-E01; B04-N04; B11-C08A; B11-C09E4; B12-K04; S05-H18A

EPI: S03-E10A3; **S03-E14H5**; **T01-J08A2**; V05-J01A

TECH UPTX: 20021010

TECHNOLOGY FOCUS - BIOTECHNOLOGY - Preferred Method: In M1, the oligomer from MSD of fragments is used. The second ranking is also calculated and the a cumulative ranking, based on first and second ranking, for each sequence of a set of fragment sequences having at least the second number of monomers is calculated. The terminal portion of the protein is a N-terminus, C-terminus and 3'terminus. The label which is attached to the terminal portion is covalently bonded to the protein to generate the mass spectrum data and the mass spectrum data is transformed from an output of a detector plate. The protein is fragmented by collision-induced dissociation to generate fragments, which are accelerated towards a detector plate to generate the mass spectrum data. The protein is isolated from other proteins extracted from a sample, where the method involves a digital processing system which executes computer programming instructions. PDS comprises all possible m/z values empirically found in mass spectra for all possible amino acid sequences having a number of amino acids from one amino acid to a selected number of amino acid, the selected number is in a range from 4-6 amino acid. PDS comprises a set of

fragments and a set of ionic charge states. The method is performed for each protein in a set of proteins extracted from a biological material and where the set of proteins are more than 100 different proteins. In M3, the first abundance parameters and the ranking for the sequence are stored in temporary volatile cache memory. The m/z values is calculated as needed rather than stored on a non-volatile storage device. The ranking for the sequence is determined from the first abundance parameters and the abundance values obtained in the second readout operation, and where the temporary volatile cache memory comprises at least one of an L1 and an L2 cache of a microprocessor. The label is covalently bonded to a primer sequence of a nucleic acid prior to the fragments being generated by Sanger, polymerase chain reaction, or Maxam-Gilbert methods and the generation of mass spectrum data. In M4, one or more labels are used. The label incorporates one or more elements with an atomic number between 17 and 77, excluding S and P. The mass defect elements of the label have an atomic number between 35 and 63.

ABEX UPTX: 20021010

EXAMPLE - A high mannose type oligosaccharide was sequenced. The mass defect label 2-amino-6-iodo-pyridine (Label 1) was conjugated to the reducing terminus of the oligosaccharide in the presence of sodium cyanoborohydrin (NaBH3CN). This incorporated a single mass defect element (I) into the parent oligosaccharide. The addition of the mass defect element allowed the labeled oligosaccharide fragments to be distinguished from unlabeled fragments and matrix ions in the mass spectrum. The Label 1 conjugated oligosaccharide was then aliquoted. The reactions were allowed to proceed to completion. Upon completion, the reaction products were subsequently conjugated at the reducing ends of the fragments generated by reaction with the mass defect labels shown for each enzyme alpha-mannosidase I, alpha-mannosidase, alpha-mannosidase II, beta-mannosidase, beta-hexosaminidase and N-acetyl beta-hexosaminidase in the presence of sodium cyanoborohydrin. Since these labels contain different numbers of mass defect elements, the digested fragments may be distinguished from the terminal fragment of the original oligosaccharide. An aliquot of the Label 3 conjugated reaction mixture (i.e. digested with enzyme alpha-mannosidase II is further digested with enzyme 1. The reaction reducing sugar termini generated by this reaction were subsequently conjugated to Label 2. Aliquots from all these reactions were then mixed, acidified by the addition of a 50 : v/v mixture of 2 acetic acid in methanol and subjected to mass spectral analysis. Alternatively, a different label series that incorporated a hard charge (e.g. an N-alkyl-iodo-pyridium series) could be subjected to mass spectral analysis without acidification. The resulting mass spectrum was deconvolved to remove all chemical noise that does not contain a mass defect labeled peak. The resulting deconvolved mass defect spectrum was then algorithmically searched by predicting all the possible oligosaccharide sequences that could be attached to each mass defect label used. The search algorithm calculated the mass for every branch combination of hexose (Hex), and N-acetylaminohexose (HexNAc). The mass ladder formed the fragments conjugated to Label 1 suggested that the outermost sugars must be hexoses. Since the highest mass fragment conjugated to label 1 must correspond to the parent oligosaccharide, then it was deduced that the 4 hexose mass difference to the first label 1 conjugated fragment must correspond to 4 alpha-mannoses since both enzyme 1 and enzyme 3 only cleaved alpha-mannoses. The next fragment in the label 1 mass ladder differed by an addition 4 hexoses from the previous fragment. This must correspond to a sample digested with enzyme 2. The only matching label 3 conjugated fragments were hexose fragment, F (1 2 hexose fragment) and G (a 3 hexose fragment). Since peaks F and G total 5 hexoses, it was deduced that at least one of these fragments must contain a 1 - 2 linked mannose. Since enzyme 3 only cleaves 1-3 and 1-6 linkages, therefore it was further deduced that there must be at least two separate 1-6 linked mannoses in the structure and that these mannoses must be interior to the 4 1 alpha linked mannoses. From this information it was deduced the following

partial sequence: (Man4-1 alpha 2)-(Hex..,Man_-1 alpha ?,6)-(HexNAC2,Hex1)-r where r indicates the reducing end of the oligosaccharide. This process was repeated with different enzymes until the complete sequence was determined. For e.g. digestion with enzyme alpha-mannosidase II followed by enzyme beta-mannosidase allowed the determination that the initial sequence is: -Man-1 beta 4-(HNAC2)-r. The full sequence of the reducing end of the oligosaccharide was determined by reaction with enzyme alpha-mannosidase II followed by enzyme N-acetyl beta-hexosaminidase.

L90 ANSWER 3 OF 5 WPIX (C) 2003 THOMSON DERWENT
AN **2002-426317** [45] WPIX
DNN **N2002-335207** DNC **C2002-120869**
TI Determining mass of a mass altering group present in an assayed peptide and absent from a corresponding database peptide, or vice versa, involves creating mass spectrometry data and comparing it with sequence database.
DC B04 D16 **S03 T01**
IN SMILANSKY, Z
PA (COMP-N) COMPUGEN LTD
CYC 97
PI WO 2002031509 A2 20020418 (200245)* EN 46p G01N033-68 <--
PW: AT BE CH CY DE DK EA ES FI FR GB GH GM GR IE IT KE LS LU MC MW MZ NL OA PT SD SE SL SZ TR TZ UG ZW
W: AE AG AL AM AT AU AZ BA BB BG BR BY BZ CA CH CN CO CR CU CZ DE DK DM DZ EC EE ES FI GB GD GE GH GM HR HU ID IL IN IS JP KE KG KP KR KZ LC LK LR LS LT LU LV MA MD MG MK MN MW MX MZ NO NZ PH PL PT RO RU SD SE SG SI SK SL TJ TM TR TT TZ UA UG US UZ VN YU ZA ZW
AU 2002010884 A 20020422 (200254) G01N033-68 <--
ADT WO 2002031509 A2 WO 2001-IL944 20011011; AU 2002010884 A AU 2002-10884 20011011
FDT AU 2002010884 A Based on WO 2002031509
PRAI IL 2000-138946 20001011
IC ICM **G01N033-68**
ICS G16B001-37; **G06F019-00**
AB WO 200231509 A UPAB: 20020717
NOVELTY - Determining mass of a mass altering group present in an assayed peptide (AP) and absent from a corresponding database peptide (DP), and vice versa, involves treating AP with at least two digestion agents (DA) to produce products, each having many assayed fragments, obtaining mass values of the fragments, and comparing with theoretical masses of fragments obtained by treatment of DP with the respective two DA.

DETAILED DESCRIPTION - Determining (M1) mass of a mass altering group or identifying (M2) a cleavage altering sequence present in AP and absent from a corresponding DP, and vice versa, comprises:

(a) treating AP with a first DA to obtain a first digestion product comprising several first assayed fragments, and determining the mass spectrum of the digestion product to obtain one or more mass values of the individual first assayed fragments Mia;

(b) treating AP with a further DA to obtain a further digestion product comprising several further assayed fragments, and determining the mass spectrum of the digestion product to obtain one or more mass values of the individual further assayed fragments Mja;

(c) optionally repeating step (b) according to the number of different further DAs, obtaining mass values of the individual further assayed fragments Mka, Mla, Mma;

(d) optionally identifying AP, in case of a peptide not identified earlier, by a suitable protein identification method;

(e) obtaining masses Mit or Mjt of the individual theoretical fragments of DP corresponding to AP, which fragments are obtained by the theoretical digestion of DP with the first or further DA;

(f) comparing each of Mia with each database value Mit, to obtain several differences Di = Mia-Mit and discarding all Di values lower than a predetermined threshold value to give several selected differences Di'; and

(g) comparing each of Mja with each database value Mjt, to obtain several differences Dj = Mja-Mjt and discarding all Dj values lower than a predetermined threshold value to give several selected differences Dj'.

(M1) further comprises a step (h) of comparing theoretical fragments, and Di' and Dj', preferably comprising overlapping theoretical fragments, and identifying those which are essentially identical, and optionally repeating steps (e)-(h), according to the number of different further DAs, obtaining selected differences Dk'/Dl'/Dm', etc. The required mass of the mass altering group is defined by the essentially identical Di'/Dj' values. (M2) comprises repeating step (e) according to the number of different further DAs, obtaining masses Mkt, Mlt, Mmt, etc., of the individual theoretical fragments. Step (f) and (g) involves discarding all Mia/Mja and Mit/Mjt for which at least one of the Di/Dj values is lower than a predetermined threshold value and thus identifying orphan Mia/Mja that has no corresponding Mit/Mjt, and orphan Mit/Mjt that has no corresponding Mia/Mja. (M2) further comprises (after step (g)): (h) optionally repeating step (g) as above according to the number of different further DAs, and thus identifying orphan Mka, Mla, Mma, etc., that have no corresponding Mkt, Mlt, Mmt, etc., and identifying orphan Mkt, Mlt, Mmt, etc., that have no corresponding Mka, Mla, Mma, etc. (i) defining a first orphan region as the subset of the amino acid sequences of DP which includes all the theoretical fragments corresponding to orphan Mit for the first DA, defining a further orphan region as the subset of the amino acid sequences of DP which includes all the theoretical fragments corresponding to orphan Mjt for the further DA, optionally repeating this for further DAs Mkt etc., and finally defining a peptide orphan region as the intersection of the first orphan region with all further orphan regions, thus consisting of a subset of sequences of the peptide that were not identified by any of the DAs; (j) theoretically altering the amino acid sequence of the peptide orphan region, by adding, deleting or changing one or more amino acids, to obtain altered database fragments, and calculating a set of theoretical values of masses Malt of the altered fragments; (k) comparing each Malt with an orphan Mia, orphan Mja, orphan Mka, etc., and selecting those Malt of which the difference from an orphan Mia, Mja, Mka etc., is smaller than a predetermined threshold value. Malt representing the correct change is selected based on a pre-determined criterion, for e.g., confirmation by the largest number of different DAs, and thus identifying the amino acid sequence which is present only in AP or in DP as the altered database fragment contributing to the Malt.

An INDEPENDENT CLAIM is also included for a kit for determining a mass altering group and/or cleavage altering sequence of a peptide for use with mass spectroscopy, comprising two or more DAs, unit for digesting peptides with the agents, and an instruction manual.

USE - (M1) is useful for determining the mass of a mass altering group e.g. a sugar group, lipidic group, acyl group, acidic group, flavin, pyridoxal phosphate, or a group added by oxidation of sulfur in the peptide, or an amino acid sequence of one or more amino acid residues present in AP and absent from corresponding DP, and vice versa. The mass of the mass altering group that was determined is used to determine the identity of the group. (M2) is useful for identifying a cleavage altering sequence present in AP and absent from a corresponding DP (claimed). (M1) and (M2) enable to characterize the type of the mass altering group and cleavage altering sequence, determining its mass, identity, as well as its location within the amino acid sequence.

Dwg.0/4

FS CPI EPI

FA AB; DCN

MC CPI: B04-C02; B04-D05C; B04-N04; B04-N04B; B05-B01M; B06-A01; B11-C07A; B11-C08B1; B11-C08D1; B11-C08E; B11-C08E3; B11-C08E6; B12-K04; D05-A02C; D05-H09

EPI: **S03-E14H; T01-J**

TECH UPTX: 20010717

TECHNOLOGY FOCUS - BIOTECHNOLOGY - Preferred Method: DA is a chemical agent or a proteolytic enzyme, such as cyanogen bromide, trypsin, chymotrypsin, Glu-C, Lys-C, AspN, elastase or thermolysin. The amino acid sequence shared by the overlapping theoretical fragments is used to determine the identity and/or the location of the mass altering group within the amino acid sequence. In step (d), AP is identified by mass spectrometry, protein sequencing, immunoassay, chromatography, electrophoresis, protein chips or antibody chips. The predetermined threshold value is based on the experimental error of the methods and equipment involved. The essentially identical Di'/Dj' values defining the mass of the mass altering moiety may differ according to the error of the methods and equipment involved. The difference between AP and DP is due to a difference in organism strain or species, due to a database error, single nucleotide polymorphism (SNP) or signal peptide cleavage. AP and DP comprise non-identical, homolog sequences. The mass altering group or the cleavage altered sequence results from a mutation, alternative splicing, RNA editing, a post-translational modification that occurred in vivo, or a modification that occurred in vitro during sample preparation. The post-translational modification comprises acetylation, amidation, deamidation, farnesylation, formylation, geranylation, hydroxylation, methylation, myristoylation, phosphorylation or sulfation.

Preferred Kit: The kit comprises at least two proteolytic enzymes.

ABEX UPTX: 20020717

EXAMPLE - The assayed protein was identified by the standard methods as corresponding to database peptides (DPs) known as COQ7Human having the sequence: KMWDQEKDHLKKFNELMVMFRVRPTVLMPLWNVLGFALGAGTALLG. The first DA was trypsin, which selectively cleaved at the C-terminus of R and K, not before P. Theoretical digestion produced 6 fragments K; MWDQEK; DHLK; K; FNELMVMFR; VRPTVLMPLWNVLGFALGAGTALLG. The masses of the theoretical database fragments (defined as Mit) were Mit1, Mit2, Mit3, Mit4, Mit5 and Mit6, respectively. The second DA was chymotrypsin and the fragments generated were KMW; DQEKDHLKKF; NELMVMF; RVRPTVLMPLW; NVLGF; ALGAGTALLG. The masses of the theoretical fragments (defined as Mjt) were Mjt1, Mjt1, Mjt2, Mjt3, Mjt4, Mjt5 and Mjt6, respectively. The assayed peptide (AP) was modified by a post-translational modification to have modification X attached to the third amino acid W. The actual AP was treated in one reaction vessel with trypsin and in the other reaction vessel with chymotrypsin. Both digests were analysed by mass spectrometry. The mass spectrum of the trypsin digest showed: Mia3, Mia4, Mia6 and Miu (u standing for unknown). The masses Mia3, Mia4 and Mia6 of the AP were substantially identical (i.e. the difference was below a threshold value) to Mit3, Mit4 and Mit6 of the DP. However, Mia u had a mass that did not correspond to any of the fragments of the DP. The mass spectrum of the chymotrypsin digest showed: Mja2; Mja 4, Mja6 and Mja u, the first three being substantially identical to the corresponding fragments Mjt2, Mjt4 and Mjt6. Then, the two unknown masses Mia u and Mja u obtained by treatment with trypsin and chymotrypsin, respectively, were compared with each of the fragments, of the DP. Mia u was compared with Mit1-6 masses of the DP theoretically treated with trypsin, whereas Mja u was compared with Mjt1-6 of DP theoretically treated with chymotrypsin. It was found that: Mia u-Mit2 = Mja u-Mjt1 = X. Thus, X was considered to be significant, i.e., the mass of an altering moiety. Since Mit2 and Mjt1 each contributed to this identical difference giving the mass X, it was possible to determine the sequence of the fragment having a mass Mit2 (MWDQEK), and the sequence of fragment having a mass Mjt1 (KMW). The region overlapping in these two sequences was MW, and this was the sequence where the modification X was present.

L90 ANSWER 4 OF 5 WPIX (C) 2003 THOMSON DERWENT
AN **2001-356050** [37] WPIX
CR 2001-356049 [37]
DNN **N2001-258684** DNC **C2001-110490**
TI Identification of associated **cell signaling** proteins

useful to indicate common signaling pathways, uses comparison values based on data representing physical properties to identify associated pairs of proteins.

DC B04 D16 **S03**
IN **PELECH, S**
PA (UYPE-N) UNIV BRITISH COLUMBIA
CYC 25
PI WO 200138879 A2 20010531 (200137)* EN 90p G01N033-68 <--
DW: AT BE CH CY DE DK ES FI FR GB GR IE IT LU MC NL PT SE TR
W: AU CA JP NZ US
AU 2001016844 A 20010604 (200153) G01N033-68 <--
EP 1234187 A2 20020828 (200264) EN G01N033-68 <--
R: AT BE CH CY DE DK ES FI FR GB GR IE IT LI LU MC NL PT SE TR
ADT WO 200138879 A2 WO 2000-CA1378 20001117; AU 2001016844 A AU 2001-16844 20001117; EP 1234187 A2 EP 2000-979297 20001117, WO 2000-CA1378 20001117
FDT AU 2001016844 A Based on WO 200138879; EP 1234187 A2 Based on WO 200138879
PRAI US 2000-716357P 20000705; CA 1999-2290335 19991119; CA 1999-2290204 19991122
IC ICM **G01N033-68**
AB WO 200138879 A UPAB: 20021031
NOVELTY - **Cell signaling** proteins that are associated are identified by comparing pairs of proteins using comparison values based on data representing physical properties of the proteins, and identifying pairs having comparison values satisfying a condition indicative of an association.

DETAILED DESCRIPTION - The method comprises: (a) producing and storing comparison values for each pair based on data values representing physical properties of the respective proteins; and (b) identifying pairs having comparison values satisfying a condition indicative of an association between the proteins.

INDEPENDENT CLAIMS are also included for:

(1) an apparatus for conducting the method, comprising a receiver operable to receive the data values, and a processor circuit in communication with the receiver and configured to produce and store in a memory the comparison values and identify pairs as above;

(2) a computer readable medium providing instructions to direct a programmable device to conduct the method as above; and

(3) a computer data signal embodied in a carrier wave comprising code segments to direct a programmable device to receive data values, produce and store comparison values and identify proteins pairs as in the method above respectively.

USE - The method is useful to identify associations between **cell signaling** proteins (e.g. **kinases**), useful to infer that the proteins form part of a common signaling pathway and so gain further information about such signaling pathways and networks. **Cell signaling** proteins are important proteins which regulate expression and activity of proteins in cells, and operate within signaling pathways and networks which govern and coordinate all cellular functions e.g. cell metabolism or death.

ADVANTAGE - The method and apparatus can be used to measure a large number of **kinases** and **kinases** substrates in a single sample.

Dwg.0/21
FS CPI EPI
FA AB; DCN
MC CPI: B04-H01; **B04-L04**; B11-C07B4; B11-C08D1; B12-K04A; D05-H09
EPI: **S03-E14H**
TECH UPTX: 20010704
TECHNOLOGY FOCUS - INSTRUMENTATION AND TESTING - Preferred Method: Optionally, the method also comprises producing data values representing physical properties of the proteins e.g. by producing signals representative of proteins in a single dimensional electrophoreses gel. Data values are preferably normalized relative to at least one reference

value before producing comparison values, and comparison values are preferably produced and stored in a random access memory. Comparison values may be generated by: (i) receiving sets of data values representing amounts of respective **cell signaling** proteins in the biological material, and producing a coexpression coefficient for each pair, representing the degree of coexpression of the respective proteins of the pair; (ii) receiving sets of data values indicating the phosphorylation states of the respective **cell signaling** proteins in the biological material, and producing a coregulation coefficient for each pair, representing the degree of coregulation of the respective proteins of the pair; or (iii) combining the results of the coexpression and coregulation analysis to produce a linkage coefficient for each **cell signaling** protein pair, as a function of the coexpression and coregulation coefficients for the pair (e.g. by dividing coregulation coefficient by coexpression coefficient). Preferred methods for (i)-(iii) are detailed in the specification. Method (iii) optionally also comprises associating at least some of the **cell signaling** proteins with respective common signaling pathways in response to the linkage coefficients (preferred methods are detailed in the specification) and optionally producing lists of such common signal pathways. Identification as in (b) preferably comprises producing a list of: pairs of associated **cell signaling** proteins; clusters of associated **cell signaling** proteins (preferred method given in the specification); or clusters of pairs for which each member of each pair is present in at least one other pair of the group.

Preferred Apparatus: Preferably, the memory is integral, and the processor circuit is configured for preferred methods as above. Especially preferred apparatus is detailed in the specification. A measuring device which can produce the data values (e.g. a chemiluminescence imager producing signals from a single dimensional electrophoresis gel) is optionally included; electrophoresis apparatus (e.g. for sodium dodecyl sulfate polyacrylamide gel electrophoresis (SDS-PAGE)) is optionally also included.

ABEX UPTX: 20010704

EXAMPLE - None given.

L90 ANSWER 5 OF 5 WPIX (C) 2003 THOMSON DERWENT
AN **2001-356049** [37] WPIX
CR 2001-356050 [37]
DNN **N2001-258683** DNC **C2001-110489**
TI Detecting multiple groups such as kinases or kinase substrates in test sample, comprises separating proteins in sample to produce one-dimensional array, contacting array with antibodies and detecting antibodies bound to groups.
DC B04 D16 S03
IN **PELECH, S**
PA (UYBE-N) UNIV BRITISH COLUMBIA
CYC 25
PI WO 2001038877 A2 20010531 (200137)* EN 61p G01N033-573
RW: AT BE CH CY DE DK ES FI FR GB GR IE IT LU MC NL PT SE TR
W: AU CA JP NZ US
CA 2290335 A1 20010519 (200141) EN G12Q001-46
CA 2290204 A1 20010522 (200143) EN G12Q001-48
AU 2001016843 A 20010604 (200153) G01N033-573
EP 1234184 A2 20020828 (200264) EN G01N033-573
R: AT BE CH CY DE DK ES FI FR GB GR IE IT LI LU MC NL PT SE TR
ADT WO 2001038877 A2 WO 2000-CA1377 20001117; CA 2290335 A1 CA 1999-2290335 19991119; CA 2290204 A1 CA 1999-2290204 19991122; AU 2001016843 A AU 2001-16843 20001117; EP 1234184 A2 EP 2000-979246 20001117, WO 2000-CA1377 20001117
FDT AU 2001016843 A Based on WO 2001038877; EP 1234184 A2 Based on WO 2001038877
PRAI US 2000-516357P 20000705; CA 1999-2290335 19991119; CA 1999-2290204 19991122

IC ICM C12Q001-48; G01N033-573
ICS C12Q001-42; G01N033-535

AB WO 200138877 A UPAB: 20021031
NOVELTY - Detecting (M) multiple groups such as kinases or kinase substrates in a test sample comprising:
(1) electrophoretically separating proteins in the sample to produce a one-dimensional array of proteins so separated;
(2) contacting the array with antibodies such as anti-kinase (substrate) antibodies; and
(3) detecting the presence of antibodies bound to kinase (substrate) groups in the array, is new.
USE - (M) is useful for detecting multiple groups such as kinases or kinase substrates in a test sample (claimed). (M) is useful for the discovery of new protein kinases, to detect unknown proteins which can cross-react with kinase-specific antibodies, and to identify known proteins and detect new proteins that may bind with high affinity to a target protein.
ADVANTAGE - (M) has many advantages over standard 2-dimensional (2D) gel proteomic methods. (M) can be applied to any cell or tissue samples, and no prelabeling with radioisotopes is necessary, because kinase detection is based on immunoreactivity. (M) can be adapted for wide scale diagnostic applications because patterns of protein kinase expression are stable for periods of up to six hours before an organ is subjected to fractionation and freezing, providing the organ is stored during this time over ice. This procedure may be carried out within two days from start to finish when compared to the 2D gel electrophoresis which is extremely laborious, much more difficult to render and takes at least twice a time. (M) provides ability to compare multiple samples side by side, whereas the 2D gel can be used for a single sample. An advantage of (M) over other methods to examine protein-protein interactions such as the yeast two-hybrid method, is that it can detect interactions that are affected by the state of post-translation regulation of these proteins, such as their phosphorylation state.
Dwg.0/0

FS CPI EPI
FA AB; DCN
MC CPI: B04-G03; B04-G22; B04-L04; B11-C07A; B11-C08D1; B12-K04A; D05-A02E; D05-H09; D05-H11E
EPI: S03-E14H4

TECH GPTX: 20010704
TECHNOLOGY FOCUS - BIOTECHNOLOGY - Preferred Method: (M) further comprises recording one or more values representative or location of antibodies bound on the array by measuring intensity of a signal representative of an amount of antibody at a location on the array and recording a value or values representative of the intensity. Recording comprises exposing photographic material to the array and developing the photographic material to produce a record, or scanning the array to produce a record comprising a signal. The signal comprises a data structure consisting of the values, and the signal is stored in a machine readable medium. In (M), at least one protein phosphatase is added to the sample prior to separating to dephosphorylate proteins in the sample, and at least one protein phosphatase is inactivated prior to separating. At least one kinase and adenosine triphosphate (ATP) is added to the sample to phosphorylate substrates of the added kinase prior to separating, and the added kinase is inactivated prior to separating. Separation is done in a sodium dodecyl sulfate-polyacrylamide gel electrophoresis (SDS-PAGE) gel in a single dimension, where the proportions of acrylamide and bisacrylamide in the gel are selected to permit separation of phosphorylated and non-phosphorylated states of a single kinase or kinase substrate group. The proteins electrophoretically separated exclude proteins from the sample of less than about 25 kilo Dalton (kD). In (M), at least one of the antibodies comprises a polyclonal antibody mixture, and the array is transferred to a membrane prior to contacting with

antibodies. Detection comprises monitoring the presence of an antibody selectively bound to anti-kinase (substrate) antibodies, where an enzymatic reaction catalyzed by a group conjugated to the antibody selectively bound to anti-kinase substrate antibodies is monitored.

UPTX: 20010704

ABEX EXAMPLE - The presence of over 45 different protein kinases in soluble extracts prepared from the whole brain, heart and skeletal muscle of adult male Sprague-Dawley rats was probed. The results demonstrated large differences in kinase expression patterns between those tissues. Brains, hearts and hind leg tibial skeletal muscles from 50 day old male Sprague-Dawley rats were rapidly excised. The tissues were cut, rinsed with phosphate buffered saline, frozen in liquid nitrogen, and stored. The tissues were pulverized, re-suspended in ice-cold homogenization buffer and sonicated. The homogenates were ultracentrifuged and the supernatants were immediately frozen until subsequent analysis. The thawed cell lysates were measured for protein content using bradford reagent with bovine serum albumin as the reference standard. The protein concentration of the lysates was adjusted to 1 mg/ml in sodium dodecyl sulfate-polyacrylamide gel electrophoresis (SDS-PAGE) sample buffer and boiled. 1 mg of the cell lysate was loaded on to the stacking layer of an SDS-PAGE gel. Electrophoresis was performed until proteins of 25,000 Daltons had migrated to the bottom of the gel. Proteins were then electrophoretically transferred from the gel on to a nitrocellulose membrane, and the membrane was subsequently cut vertically into 1 cm wide strips. The strips were then blocked with 5% skim milk powder in Tris-buffered saline and, after quickly rinsing the membrane with TBST (undefined), each strip was exposed to a unique mixture of different primary antibodies in TBST. The strips were washed with TBST and incubated with horseradish peroxidase-conjugated secondary antibody. After washing the strips with TBST, the strips were reassembled, and subjected to the enhanced chemiluminescence (ECL) Western blotting detection system. The results showed that the patterns of kinase expression differed markedly between the tissues. At least 45 known protein kinases were visualized on the immunoblots and clearly identified based on their predicted sizes and immunoreactivities.

=> d his

(FILE 'HOME' ENTERED AT 19:00:35 ON 28 MAY 2003)
SET COST OFF

FILE 'MEDLINE' ENTERED AT 10:00:57 ON 28 MAY 2003
E PELECH S/AU
L1 151 S E3-E7
L2 51 S L1 AND L1./CT
E CELL COMMUNICATION/CT
E E3+ALL
L3 13507 S E4
L4 73022 S E22
L5 135819 S E4+NT
E E30+ALL
E SIGNAL/CT
E E52+ALL
L6 73071 S E11
L7 120317 S E11+NT
L8 40 S L1 AND L3-L7
L9 73 S L1 NOT L2,L8
L10 79 S L2,L8

FILE 'HCAPLUS' ENTERED AT 10:34:17 ON 28 MAY 2003
E PELECH S/AU
L11 166 S E3-E9
L12 2 S L11 AND P/DT

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                E INFORMATION SYSTEMS/CT
L13          6662 S E3,E8,E5,E16,E19-E21,E23,E25-E27
L14          6662 S E3-E27
                E E5+ALL
L15         11394 S E2-E7
L16          6919 S E24-E47
                E E6+ALL
L17          3947 S E1
                E MEMORY DEVICE/CT
L18          7213 S E30-E31
L19          3570 S E8
                E E4+ALL
L20         43101 S E4+NT
L21           338 S L13-L17 AND L16-L20
                E SIGNAL TRANSDUCTION/CT
                E E6+ALL
L22             2 S L21 AND E1+NT
                E E8+ALL
L23             1 S L21 AND E4+NT
L24            77 S L21 AND (BIOCHEM?(L)METHOD?)/SC,SX
L25            25 S L21 AND SIGNAL?
                E PHYSICAL PROPERT/CT
L26             2 S L21 AND E4
L27            52 S L21 AND PROTEIN
L28             4 S L13,L22,L23,L26
L29            24 S L24,L25 AND L27 NOT L28
L30            89 S L24,L25,L27 NOT L28-L29
                SEL DN AN 13 13 16 18 80 82
L31             6 S L30 AND E1-E18
L32            10 S L28,L31
L33            24 S L29 NOT L30-L32
                SEL DN AN 7 8 10 11 14 19
L34             6 S L33 AND E19-E26
L35            16 S L32,L34 AND L11-L34
                E MATHEMATICAL METHOD/CT
                E E4+ALL
L36         98747 S E3-E5,E2+NT
                E E123+ALL
L37         36824 S E2,E1+NT
L38        150770 S E9+NT OR E14+NT OR E15+NT OR E16+NT
L39            92 S L21 AND L36-L38
L40            11 S L39 AND L35
L41            16 S L35,L40
L42            30 S L39 NOT L29-L35,L41
L43            16 S L41 AND L11-L42

      FILE 'HCAPLUS' ENTERED AT 11:00:09 ON 28 MAY 2003
L44             9 S L21 AND SCLUSTER?
L45             8 S L44 NOT L43
                SEL DN AN 5 8
L46             6 S L45 NOT E1-E6
L47             6 S L46 AND L11-L46

      FILE 'COMPUSCIENCE' ENTERED AT 11:04:19 ON 28 MAY 2003
                E RELEICH/AU
                E RANDOM ACCESS/CC
                E MEMORY/CC
L48          5527 S E3
                E RANDOM ACCESS/ST
L49          3961 S RANDOM?/ST
L50           110 S L48 AND MEMORY?/CC,ST
L51             0 S L50 AND (PROTEIN OR PEPTIDE OR POLYPEPTIDE OR NUCLEIC ACID OR
L52             6 S L46 AND (PROTEIN OR PEPTIDE OR POLYPEPTIDE OR NUCLEIC ACID OR
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                SEL DN AN 6
L53               1 S L52 AND E1

     FILE 'COMPUSCIENCE' ENTERED AT 11:08:08 ON 28 MAY 2003
L54             767 S MEMORY DEVICES/ST
L55            5527 S MEMORY?/CC
L56            5530 S L54,L55
L57               6 S L56 AND (PROTEIN OR PEPTIDE OR POLYPEPTIDE OR NUCLEIC ACID OR
L58              12 S L56 AND CELL?(L)SIGNAL?
L59              12 S L57,L58 NOT L52

     FILE 'COMPUAB' ENTERED AT 11:09:59 ON 28 MAY 2003
                E MEMORY/CC
                E BIO/CC
L60            8711 S E4-E27
L61             204 S L60 AND MEMOR?
L62              12 S L61 AND RANDOM?
L63            2694 S RANDOM? ACCESS?
L64              11 S L63 AND L60
L65               7 S L64 NOT L62
L66            1624 S L63 AND STOR?
L67             200 S L66 AND SIGNAL?
L68               2 S L60 AND L67
L69              37 S L67 AND CELL?

     FILE 'WPIX' ENTERED AT 11:14:05 ON 28 MAY 2003
                E PELECH S/AU
L70               4 S E3
                SEL DN AN 1 2
L71               2 S L70 AND E1-E6
L72           71267 S G01N033-6?/IC,ICM,ICS
L73            1064 S L72 AND (M423 OR M740)/M0,M1,M2,M3,M4,M5,M6
L74             834 S L73 AND (N180 AND N233)/M0,M1,M2,M3,M4,M5,M6
L75             276 S L73 AND (N102 AND N136)/M0,M1,M2,M3,M4,M5,M6
L76             408 S L73 AND (N102 AND N135)/M0,M1,M2,M3,M4,M5,M6
L77             845 S L74-L76
L78              21 S L77 AND G06F/IC,ICM,ICS
L79              21 S L77 AND T?/MC
L80              21 S L77 AND T?/DC
L81               0 S L77 AND G06T/IC,ICM,ICS
L82             715 S L77 AND S03/DC
L83             705 S L77 AND S03-E14H?/MC
L84              18 S L82,L83 AND CELL? SIGNAL?
L85              41 S L82,L83 AND ?KINASE?
L86              19 S L82,L83 AND (B04-L04 OR C04-L04)/MC
L87               2 S L82,L83 AND (B04-B02C4 OR C04-B02C4)/MC
L88              85 S L71,L75-L80,L84-L87
                SEL DN AN 17 19 28 54
L89               4 S L88 AND E7-E18
L90               6 S L71,L89 AND L70-L89

     FILE 'WPIX' ENTERED AT 11:26:40 ON 28 MAY 2003
                SEL DN AN L71

     FILE 'HPCI' ENTERED AT 11:27:36 ON 28 MAY 2003
L91               0 S E19-E24
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